Scientific Visualization with VisIt

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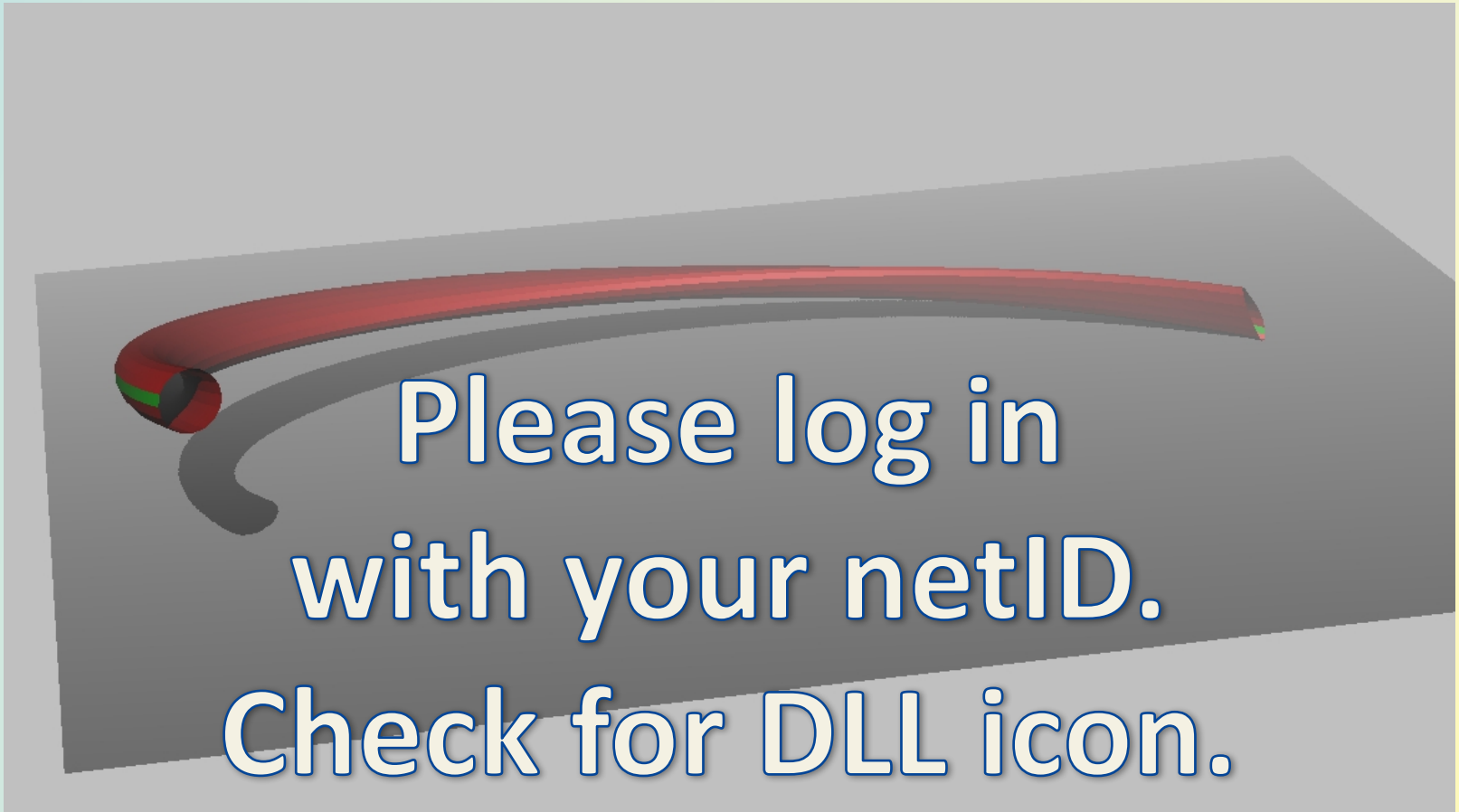


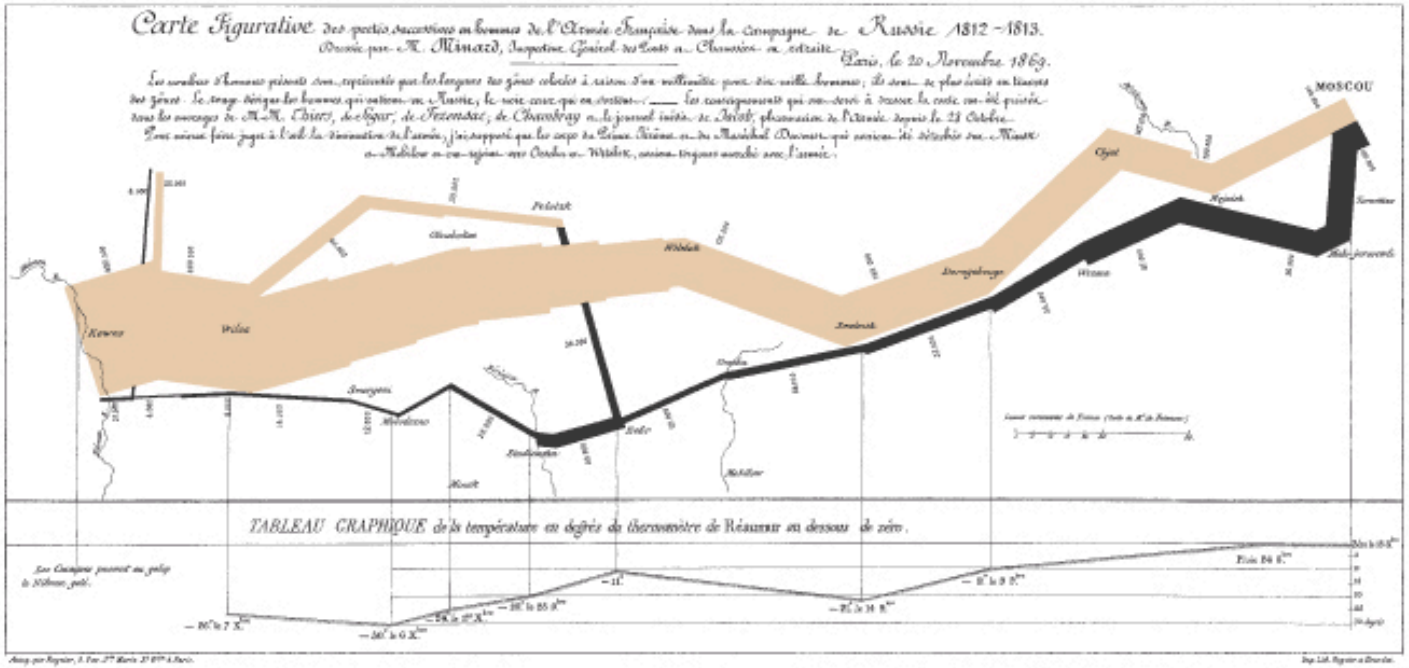
Teaching Assistants

Nelson Lin

Kyle Lui

Early Multivariate Data Vis

Not so good for Napoleon in 1812



Napoleon's March to Moscow The War of 1812

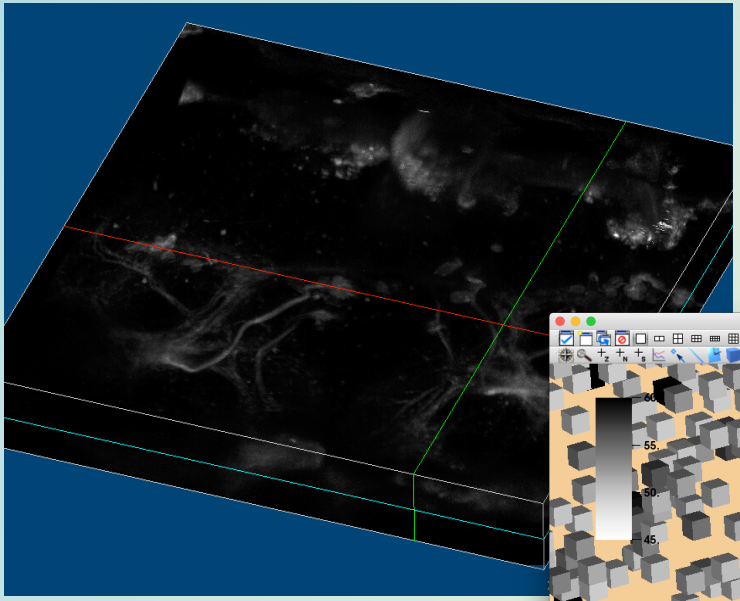
Charles Joseph Minard

This classic of Charles Joseph Minard (1781–1870), the French engineer, shows the terrible fate of Napoleon's army in Russia. Described by E. J. Marey as seeming to defy the pen of the historian by its brutal eloquence, this combination of data map and time-series, drawn in 1869, portrays the devastating losses suffered in Napoleon's Russian campaign of 1812. Beginning at the left on the Polish-Russian border near the Niemen River, the thick band shows the size of the army (422,000 men) as it invaded Russia in June 1812. The width of the band indicates the size of the army at each place on the map. In September, the army reached Moscow, which was by then sacked and deserted, with 100,000 men. The path of Napoleon's retreat from Moscow is depicted by the darker, lower band, which is linked to a temperature scale and dates at the bottom of the chart. It was a bitterly cold winter, and many froze on the march out of Russia. As the graphic shows, the crossing of the Berezina River was a disaster, and the army finally straggled back into Poland with only 10,000 men remaining. Also shown are the movements of auxiliary troops, as they sought to protect the rear and the flank of the advancing army. Minard's graphic tells a rich, coherent story with its multivariate data, far more enlightening than just a single number bouncing along over time. Six variables are plotted: the size of the army, its location on a two-dimensional surface, direction of the army's movement, and temperature on various dates during the retreat from Moscow. It may well be the best statistical graphic ever drawn.

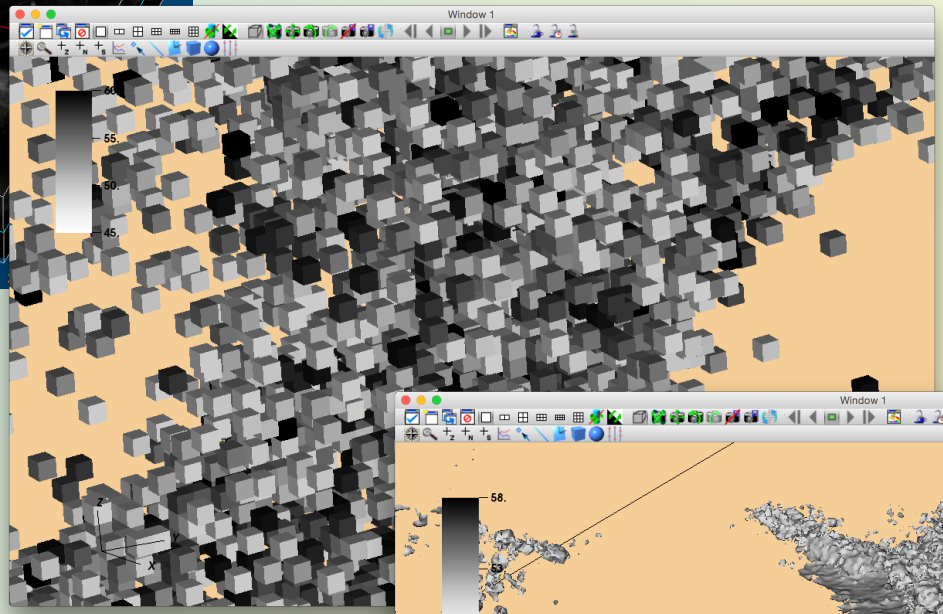
Edward R. Tufte, The Visual Display of Quantitative Information Graphics Press, Box 430 Cheshire, Connecticut 06410

Credit: Edward Tufte via Charles Minard 1869

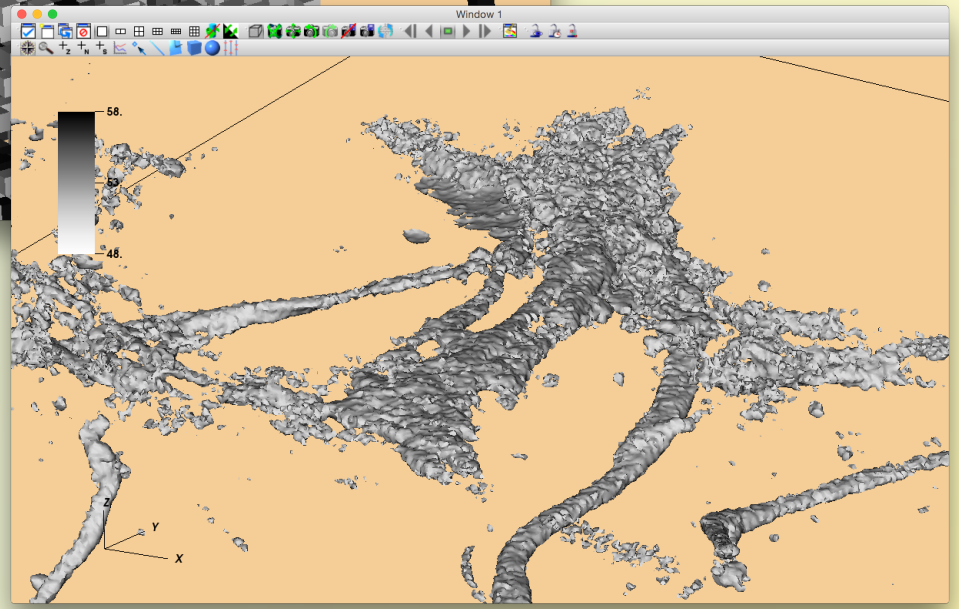
Acquire



Analyze



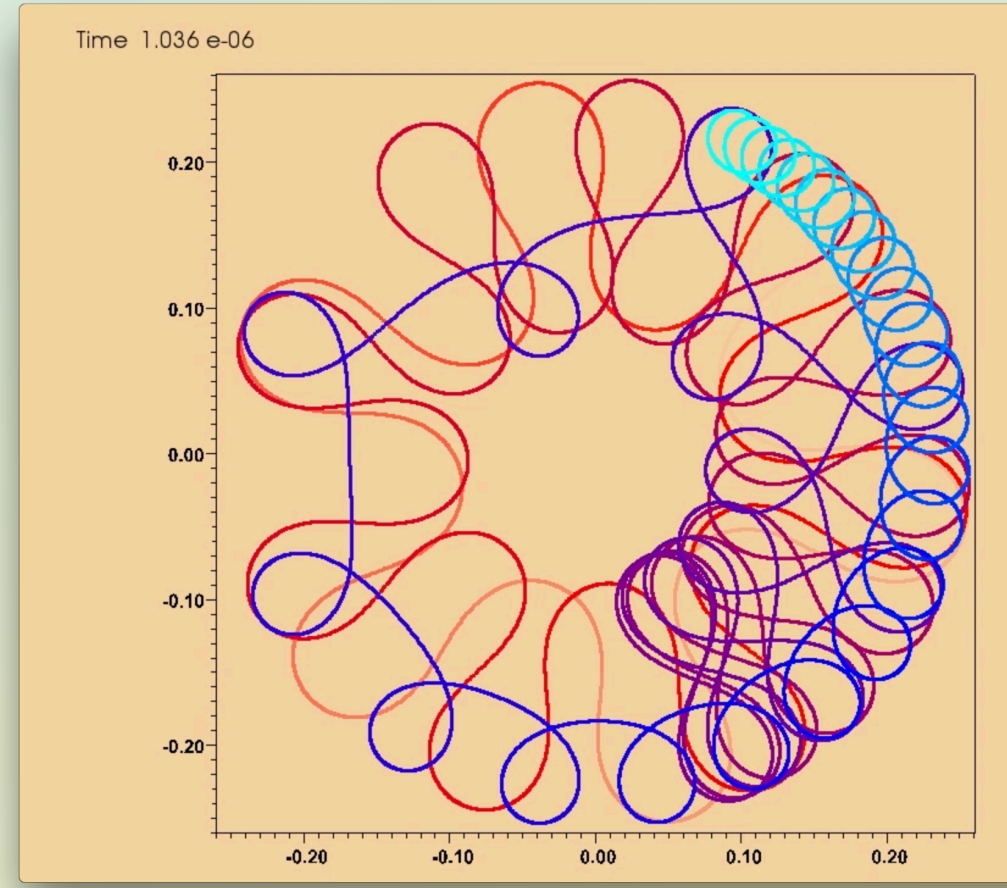
Visualize



Work Flow

Visualization of 1 Particle Can Be Interesting:

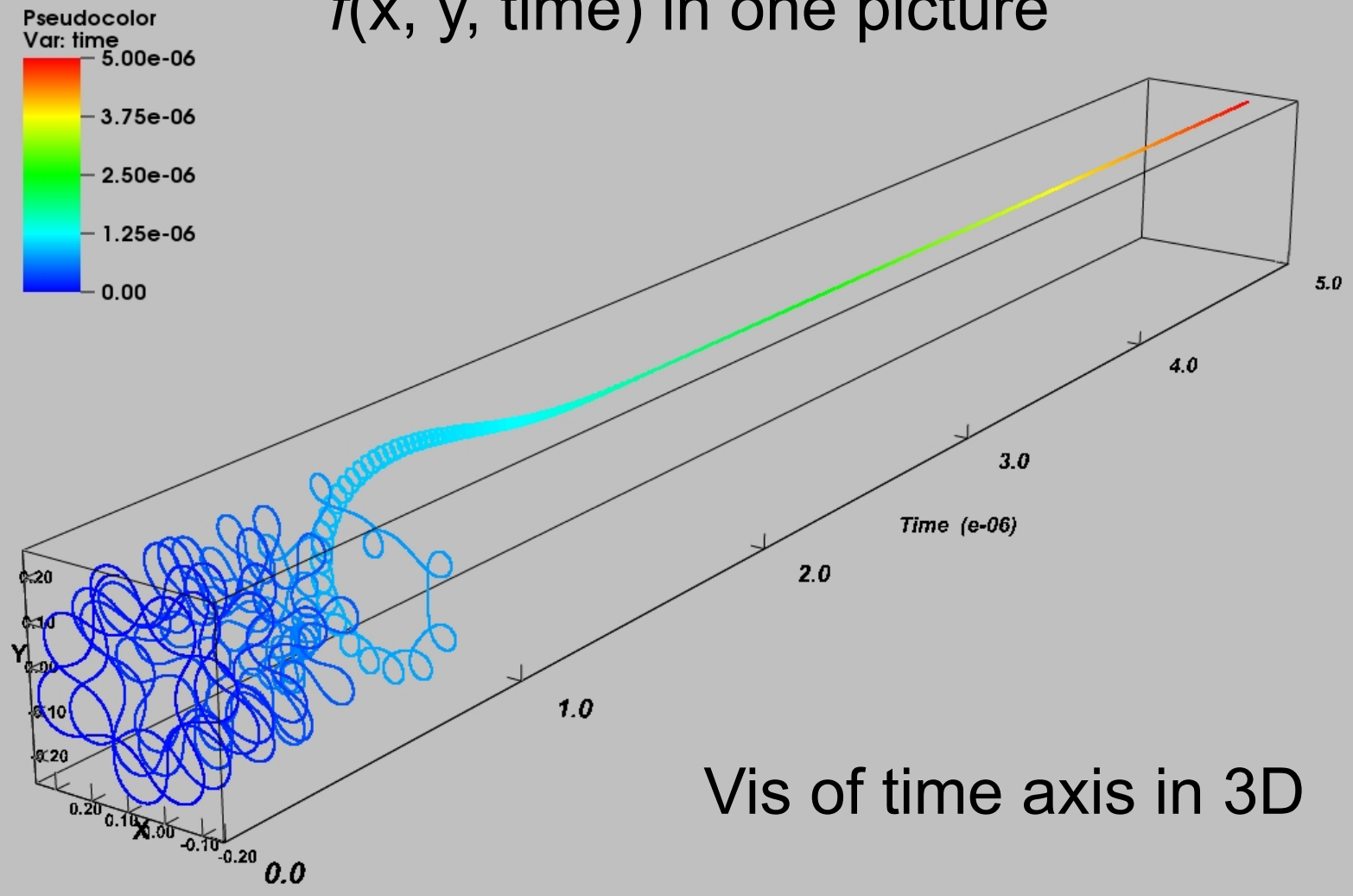
Simulation of Ion Path as Energy Decreases



Trajectory starts as betatron.
Transitions to Figure 8.
Finally becomes cyclotron.

http://w3.pppl.gov/~efeibush/movies/m3_720.mov

Visualization of 1 Particle



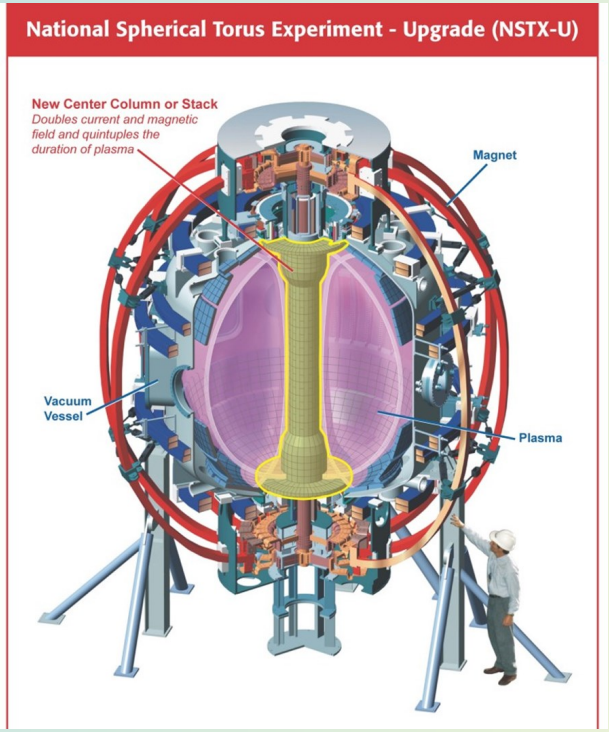
f(x, y, time) in one picture

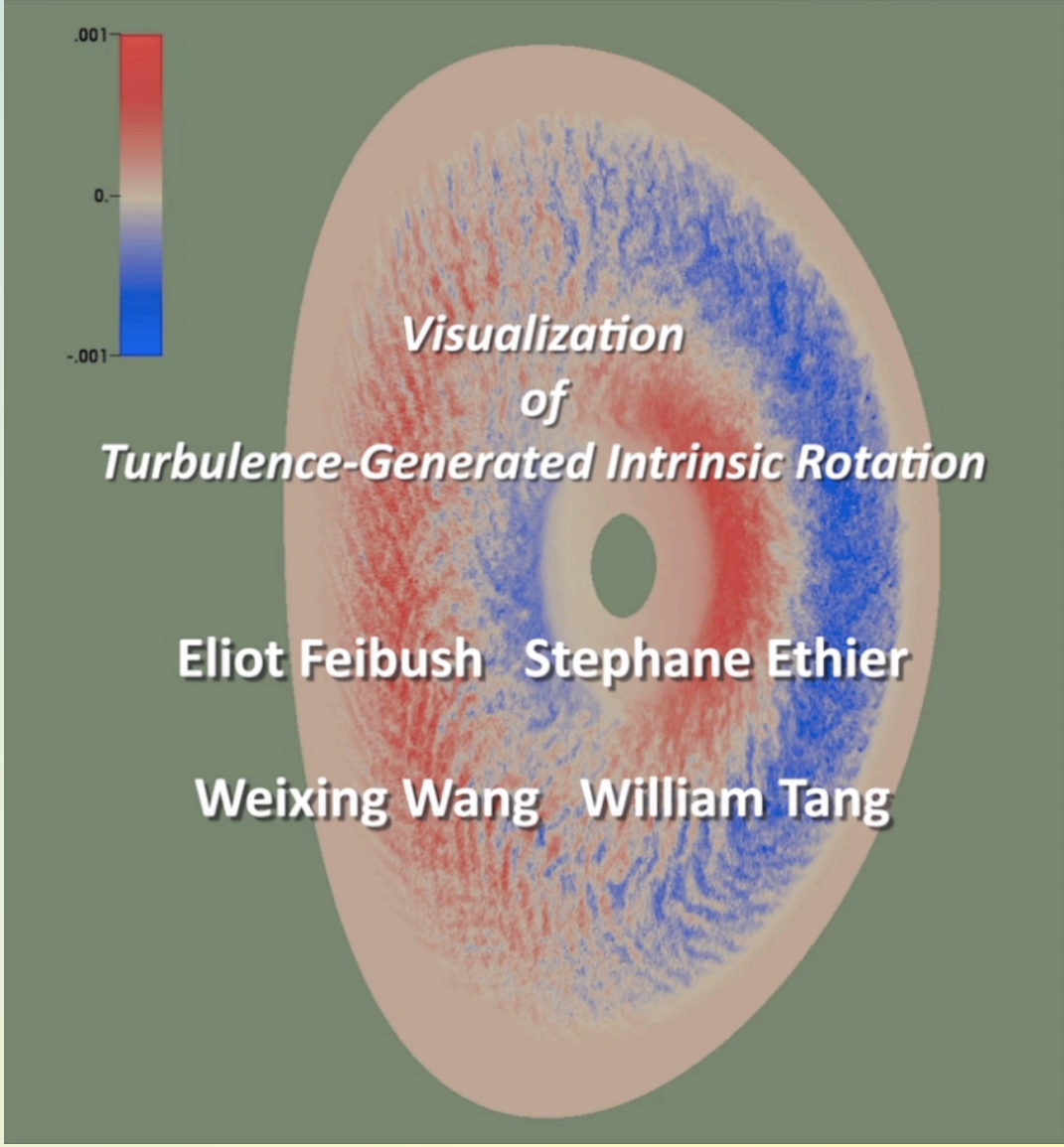
Vis of time axis in 3D

Time Step Simulation

Render each time step to a JPEG image.

Combine images to create animation.

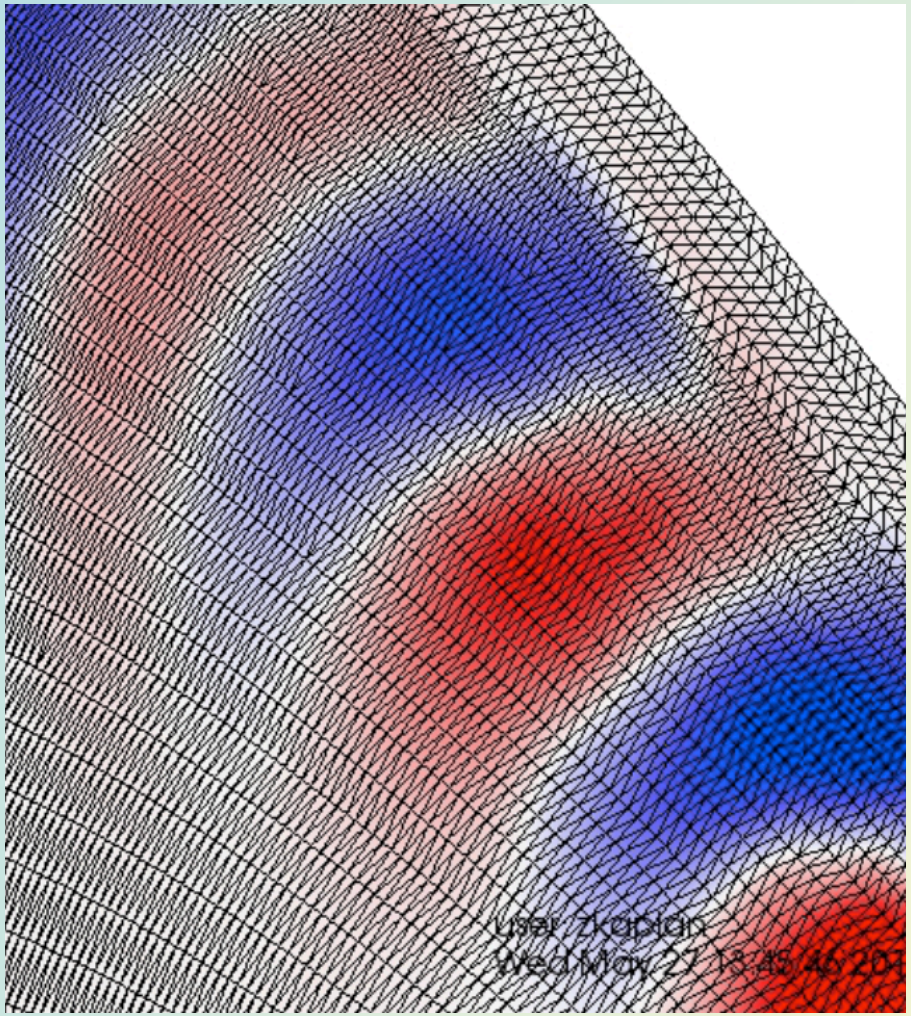


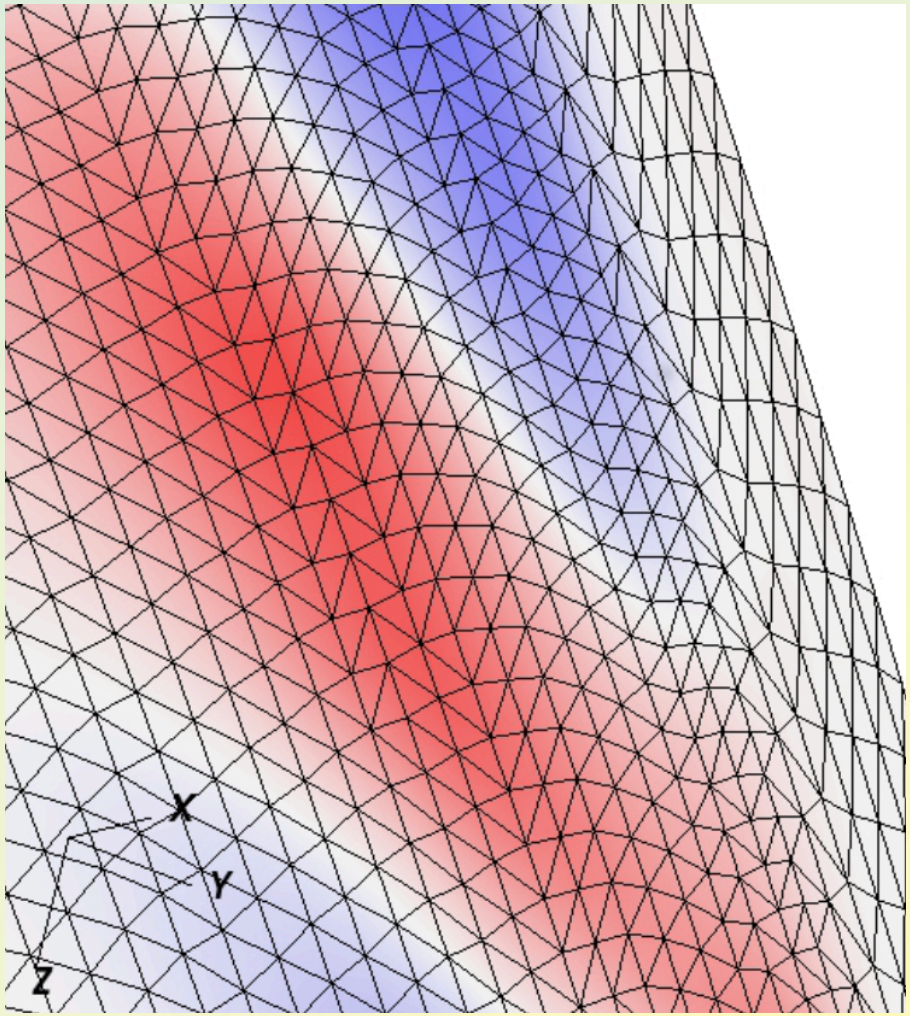


http://w3.pppl.gov/~efeibush/movies

tfden.mov

GTS Complex Grid – Poloidal Rings





Gaining insight …

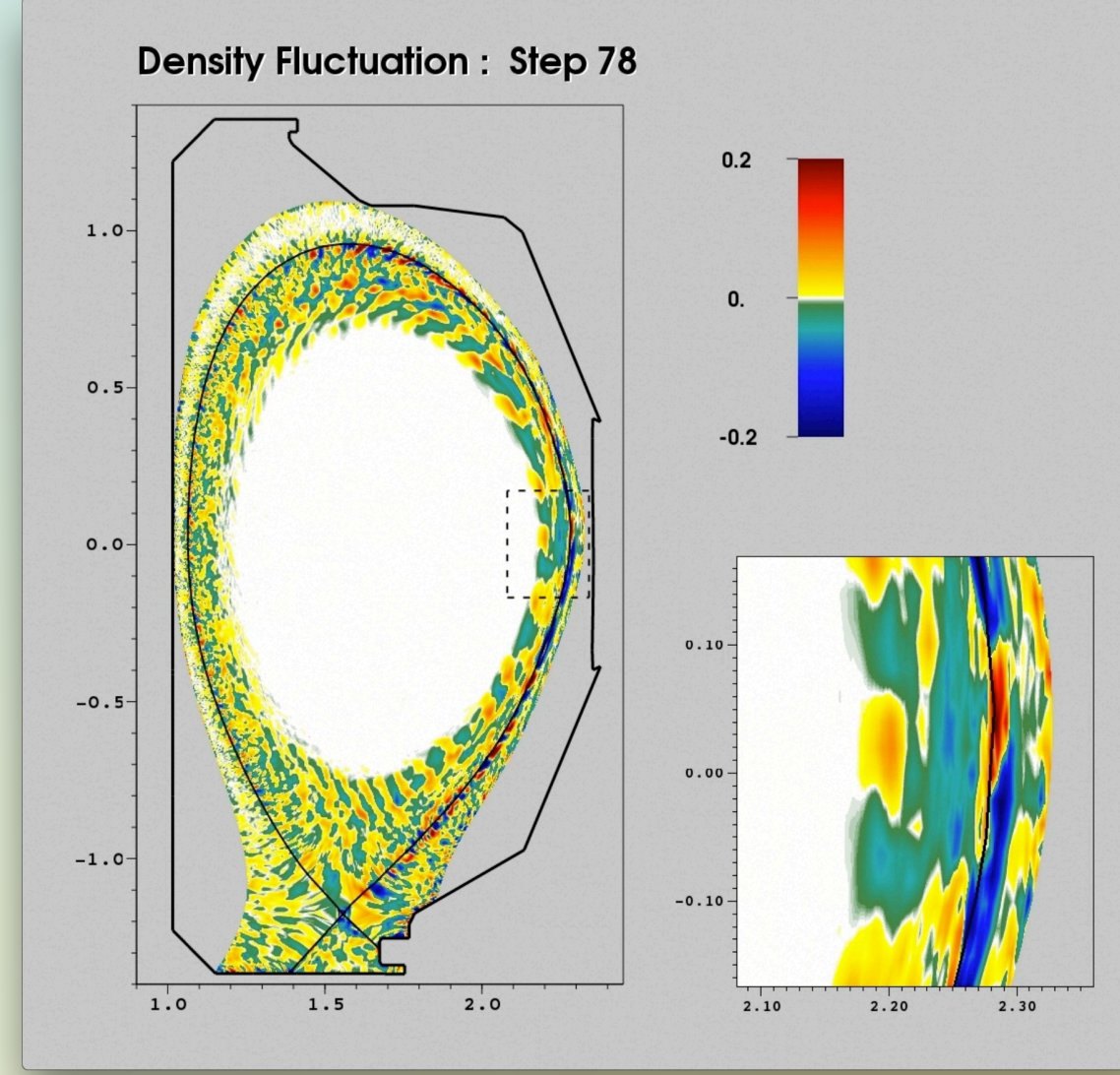
Time Step Simulation

Render overview

+

Region of Interest

Combine images into movie.



http://w3.pppl.gov/~efeibush/movies

deninsetb1080.mov

Scientific Visualization

Simulations generate data

Acquire data from experiments

- Biology
- Chemistry
- Physics
- Engineering
- ...

Explore

Communicate

Based on computer graphics

- points
- lines
- polygons, surface mesh
- 3D transformations
- hidden surface removal
- shading
- lighting

Vis Plot Types
(Based on graphics primitives)

Points

Lines

Vectors

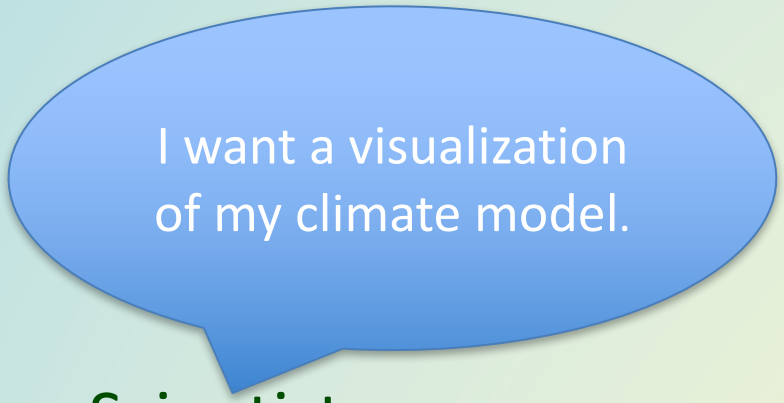
Contour lines & isosurfaces

Polygons, mesh

Volume

Molecule

Designing a Visualization



Scientist

Vis Guy

2-D/3-D Compute grid:

scalar or vector

per point, per cell

Selection + Operators

Getting to Know Your Data

Geometric range

Numerical domain (min, max)

- Histogram
- Outliers
- Features
- Local / Global (steps)

Data Science / Science of Data

n-Dimensions of Data

f(x)

f(x, time) f(x, i)

f(x, y)

f(x, y, time)

f(x, y, z)

f(x, y, z, time)

Understanding Complexity !

Time dependent data is a good candidate for animation.

VisIt Can Read Data Files

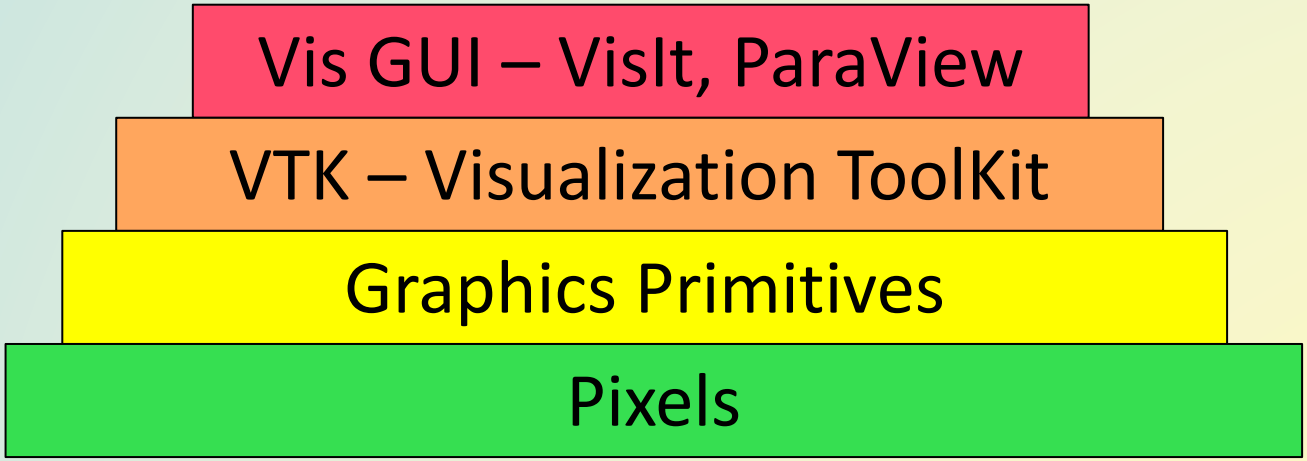
- Silo
- Chombo
- GTC
- M3D
- H5Nimrod
- SAMRAI
- S3D
- Enzo
- ITAPS
- XDMF
- Exodus
- FLASH
- EnSight
- VTK **VTK is Internal Format**
- NetCDF
- CGNS
- NASTRAN
- TecPlot
- Protein Databank (PDB)
- Plot3D
- GIS (ESRI Shapefile, DEM, many more)
- Image formats

Variable types

- Scalar
- Vector
- Tensor
- Arrays
- Label
- Material
- Species
- X,Y pairs

Database reader plug-ins can be developed for new formats

Implementation



Get Started

Log in with your NetID & password.

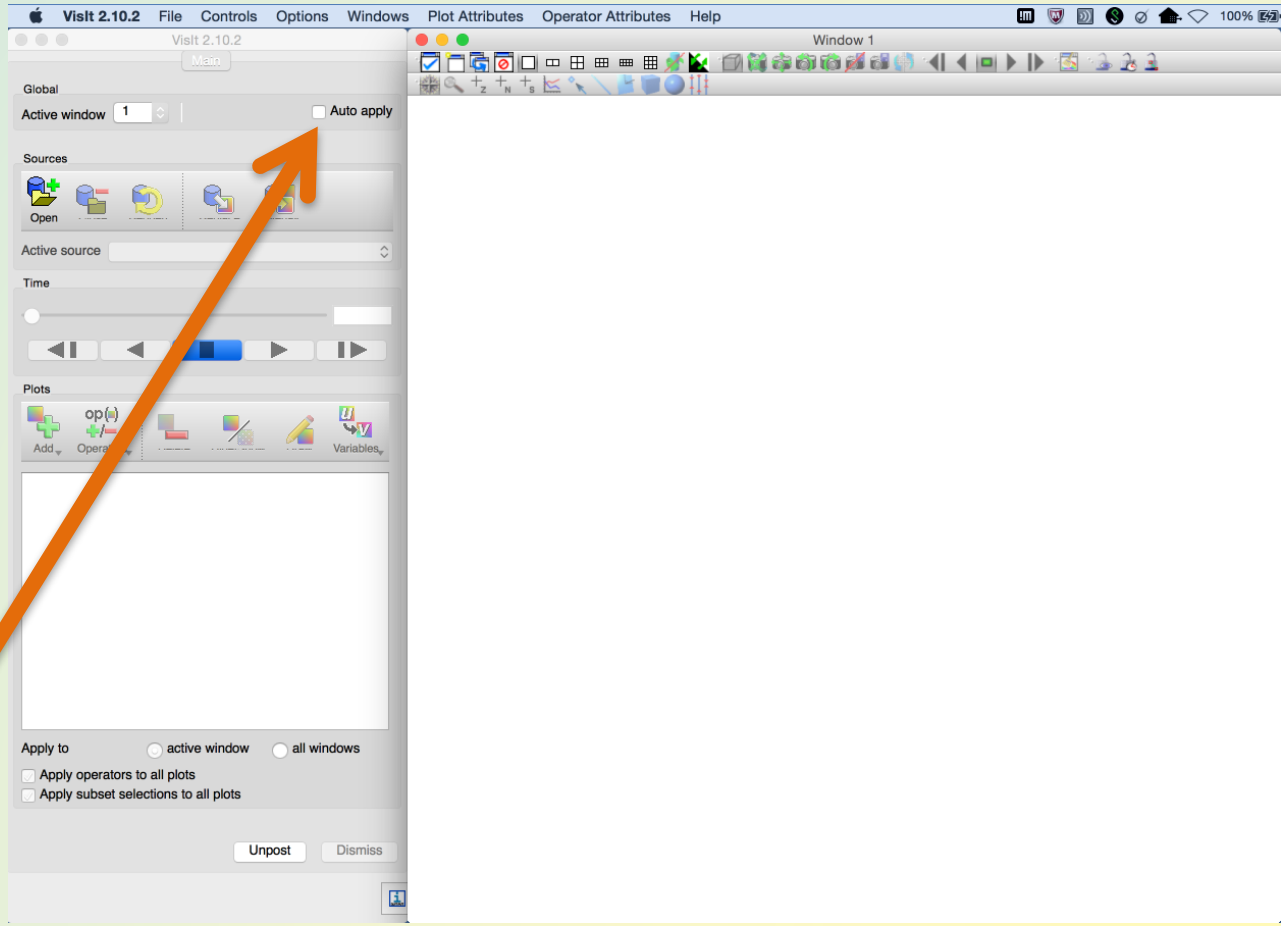
Magnifying Glass

(Spotlight Search)

visit.app

(TOP HIT - APPLICATIONS)

Check “ Auto apply”



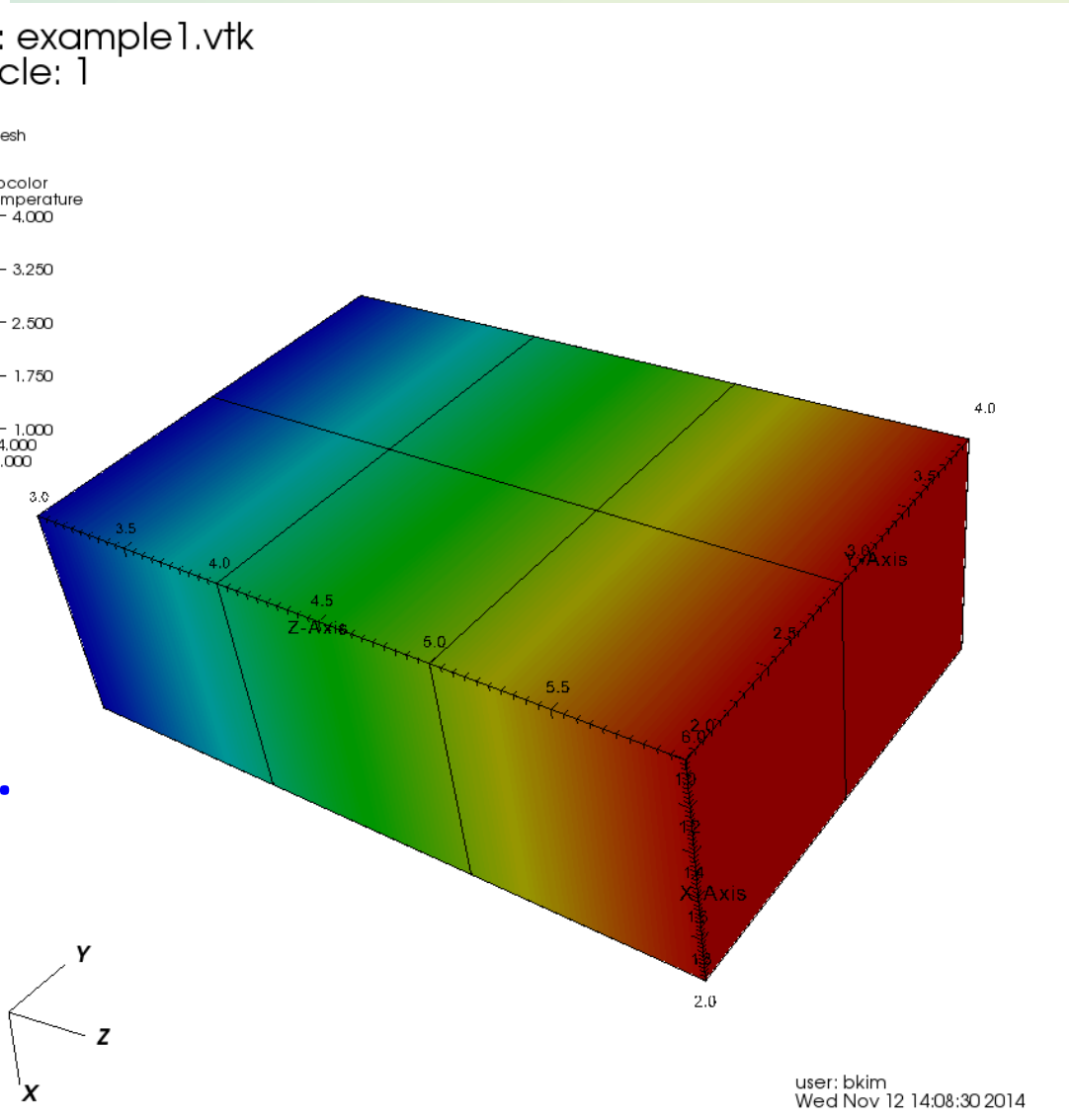
Structured Points

```
# vtk DataFile Version 3.0
VTK format
ASCII
DATASET STRUCTURED_POINTS
DIMENSIONS 2 3 4
ORIGIN 1. 2. 3.
SPACING 1. 1. 1.
POINT_DATA 24
SCALARS temperature int
LOOKUP_TABLE default
1
1
1
1
1
1
1
2
2
2
2
2
2
2
3
3
3
3
3
3
4
4
4
4
4
4
4
```

Continuous volume of data.

Uniform spacing per axis.

Value at each point.



Try It - part 1

Visit Data Files:
/Volumes/dll_drive/ViSIT DATA

reboot if not on Desktop

Open File strpts3d.vtk

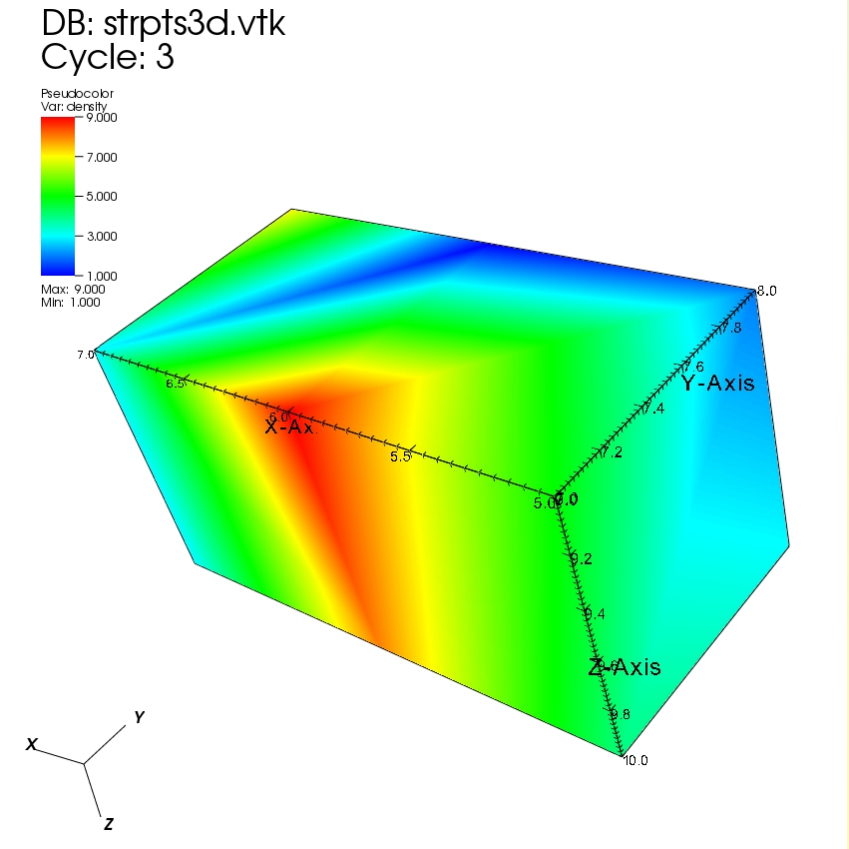
Add Pseudocolor→density

VTK:

STRUCTURED_POINTS

3 x 2 x 2 = 12 points

SCALARS density double



Continuous 3D Grids

3D volume of data

f(x,y,z)

VisIt interpolates among grid points in all 3 directions.

Specify data at grid locations.

Apply Operators to explore & examine data.

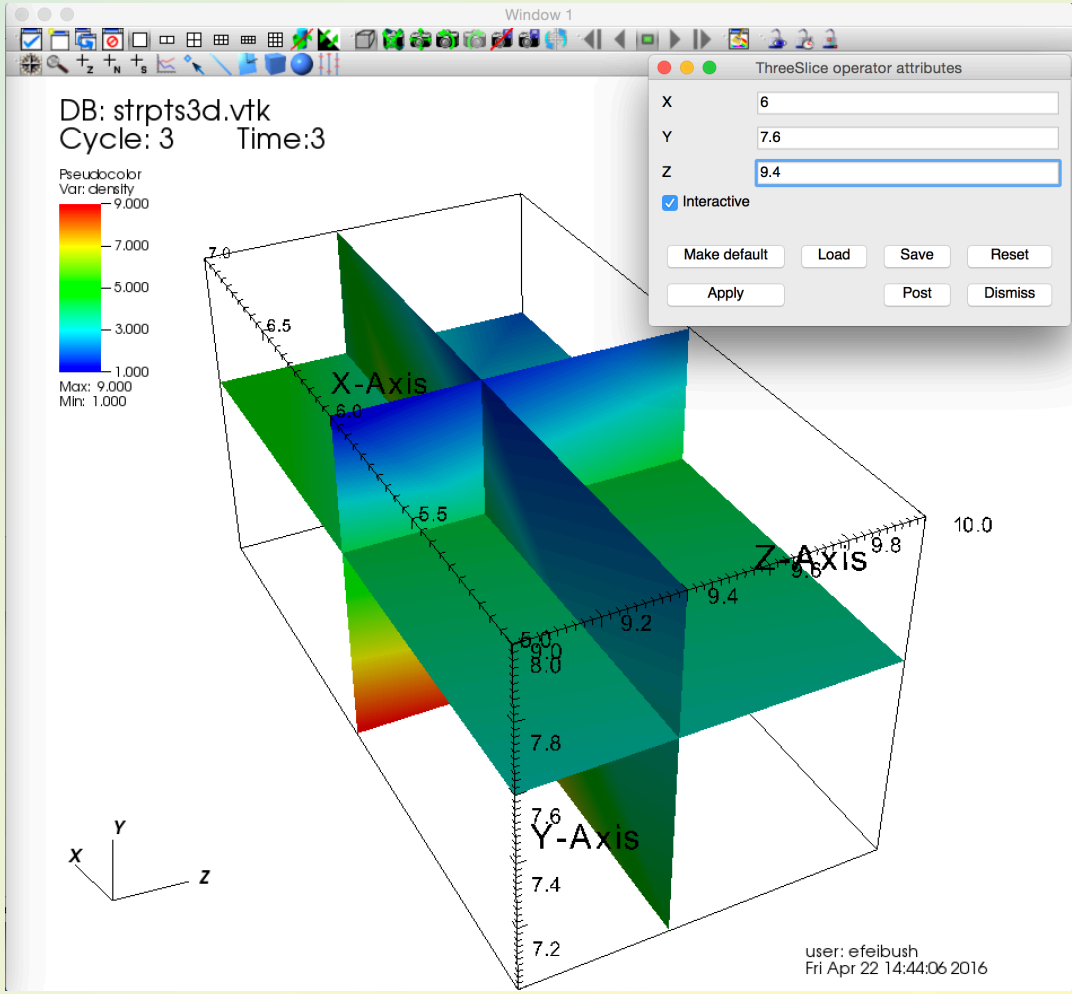
Try It - part 2

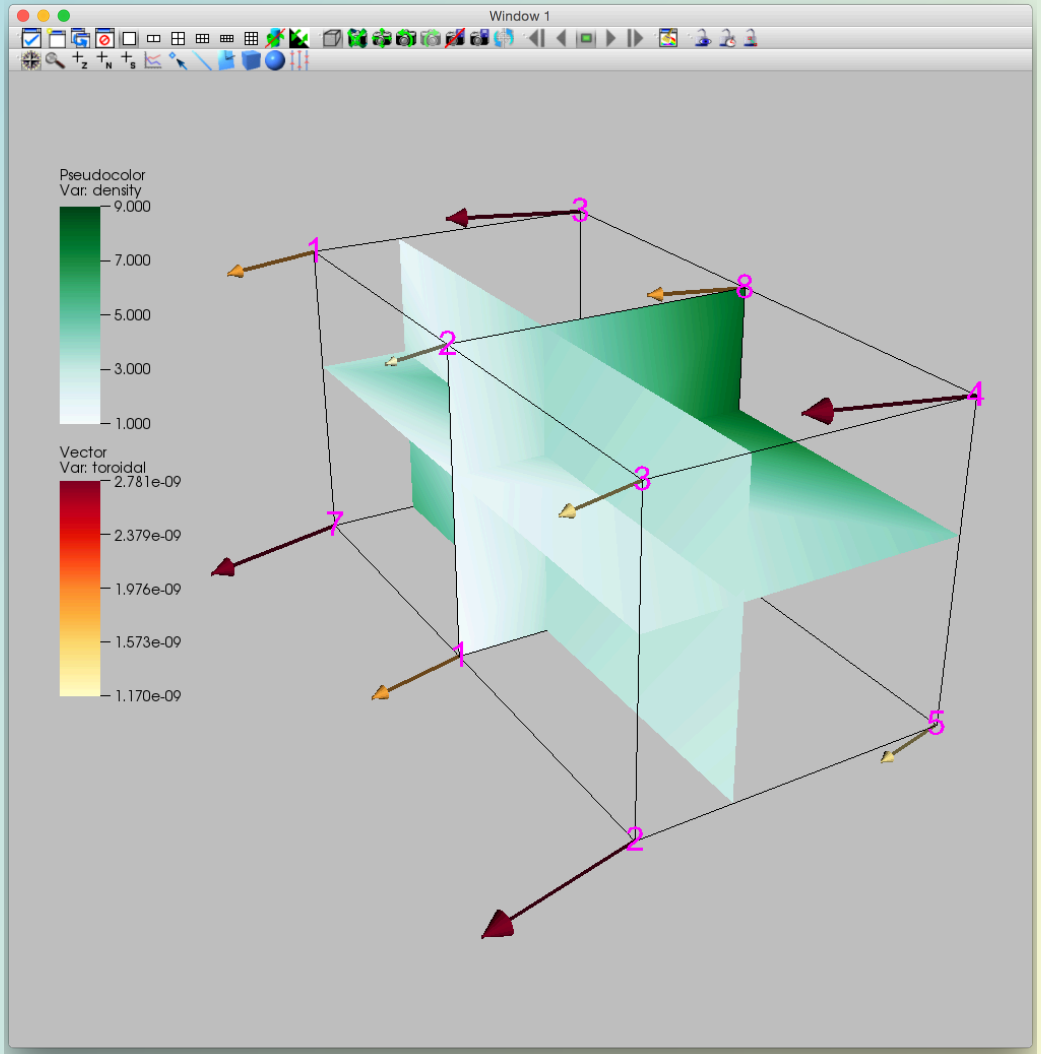
Open File strpts3d.vtk

Add Pseudocolor→density

Operators

- Slicing
  - ThreeSlice
    - X = 6
    - Y = 7.5
    - Z = 9.5





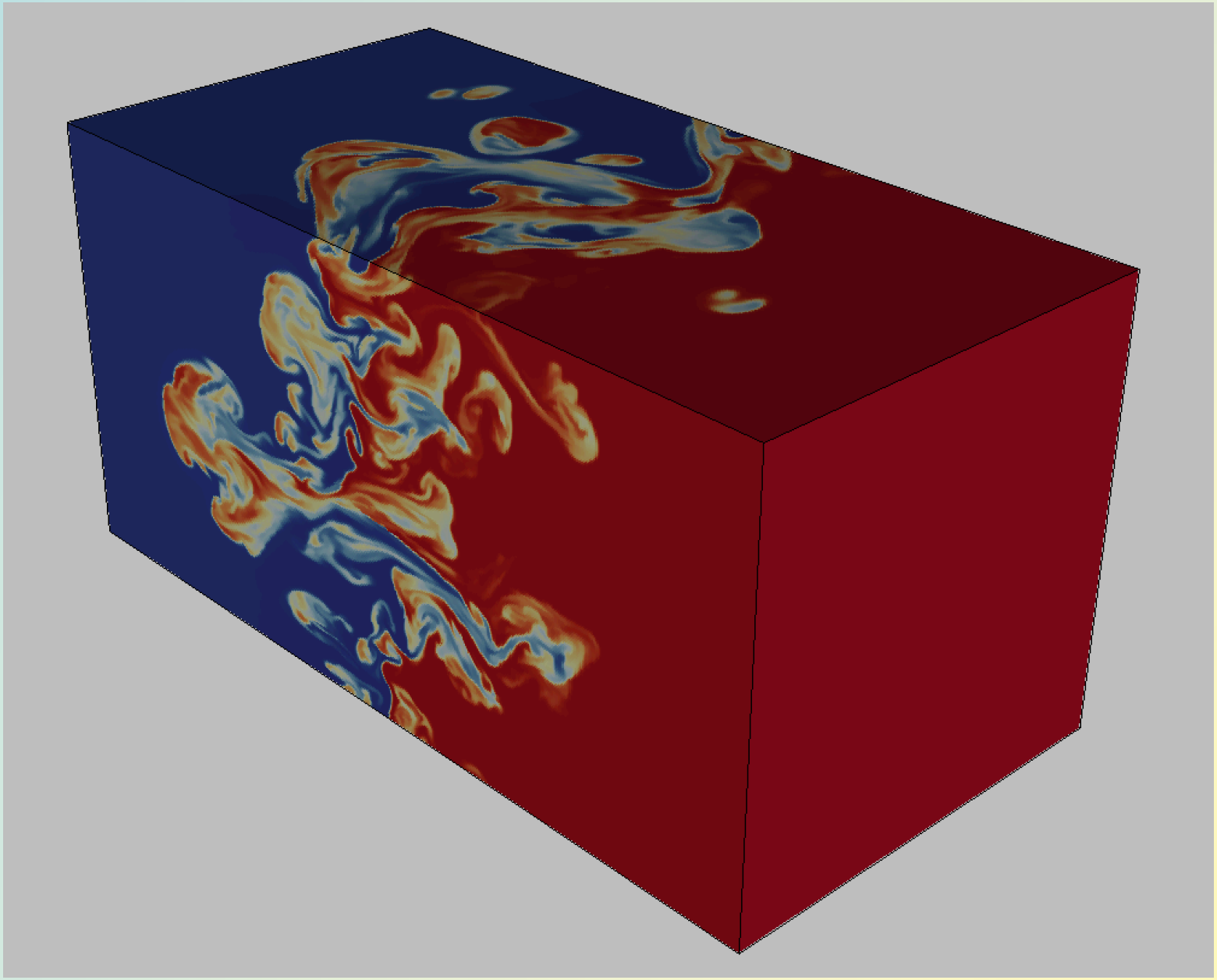
Different color maps for different variables.

Lighting – off.

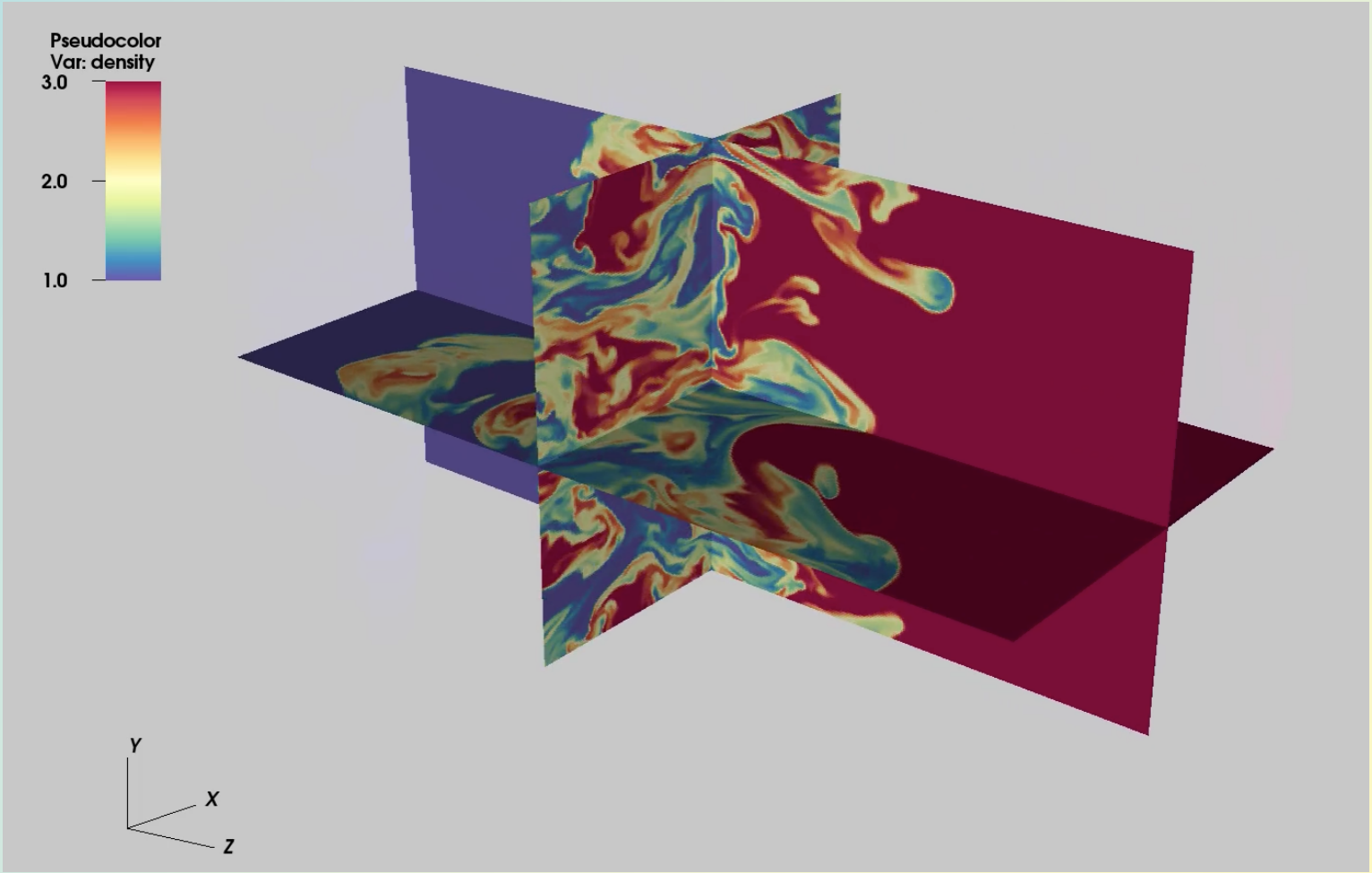
Gray background.

Density labels at mesh points.

Structured Points

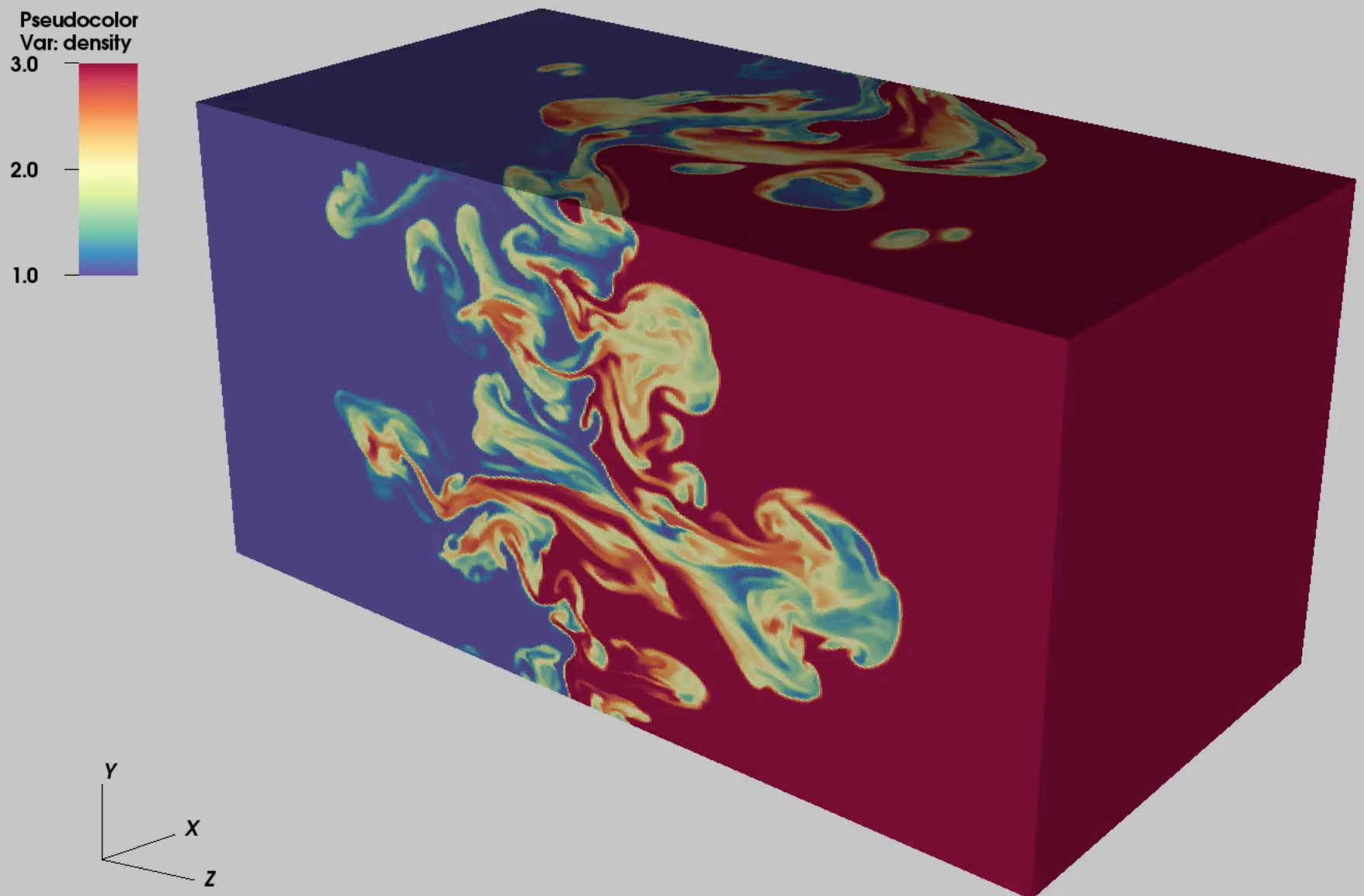


Continuous Volume of Data: Slicable



Geometric Operator: 3-Slice

Examine data throughout the volume …

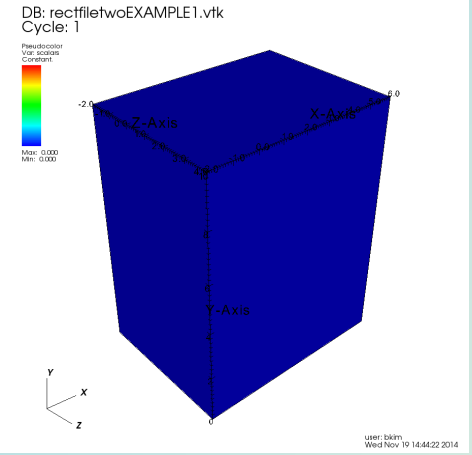

Pseudocolor
Var: density
3.0
2.0
1.0
Y
X
Z

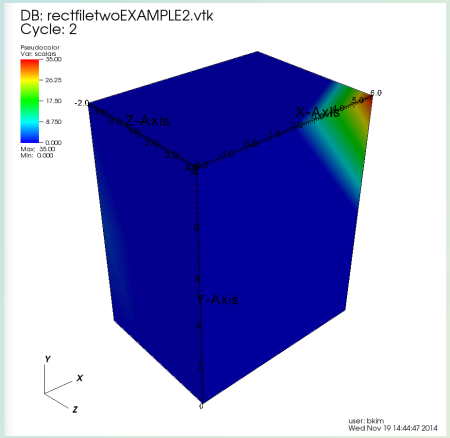
Structured Points Ordering

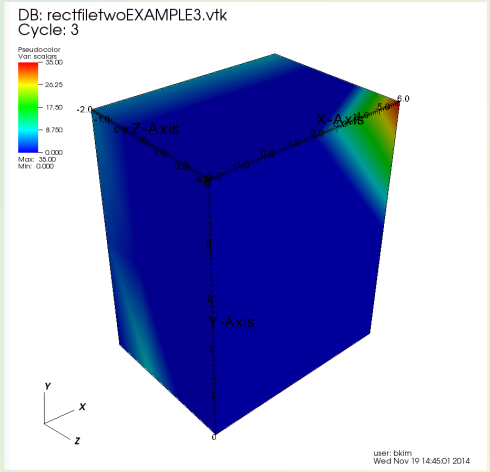
```
# Example python loop to write values
to vtk file


for z in range(4):
    for y in range(3):
        for x in range(2):
            # write f(x,y,z) value to file
```

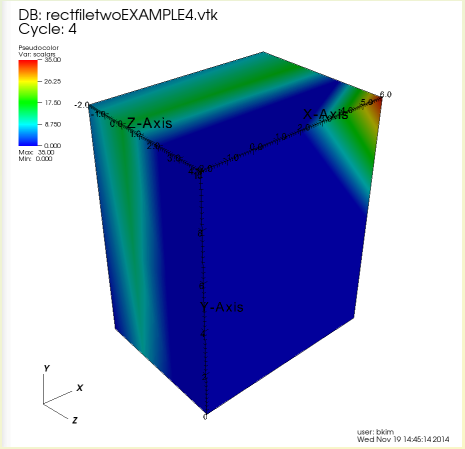
Time Steps *f(x,y,z,t)*

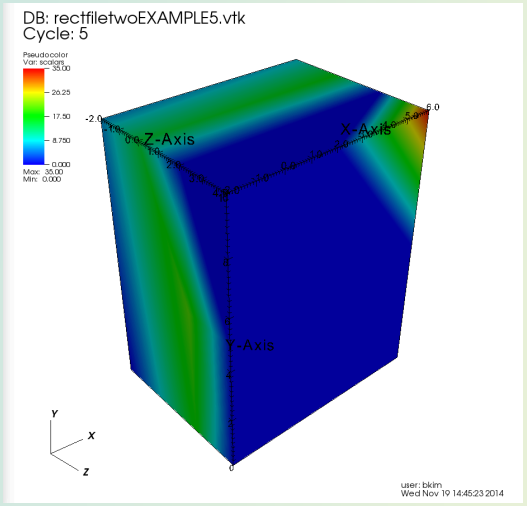
VisIt automatically reads files named in numerical order for time step visualization.

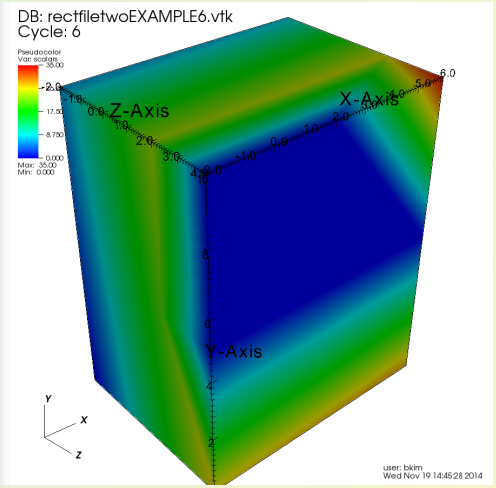


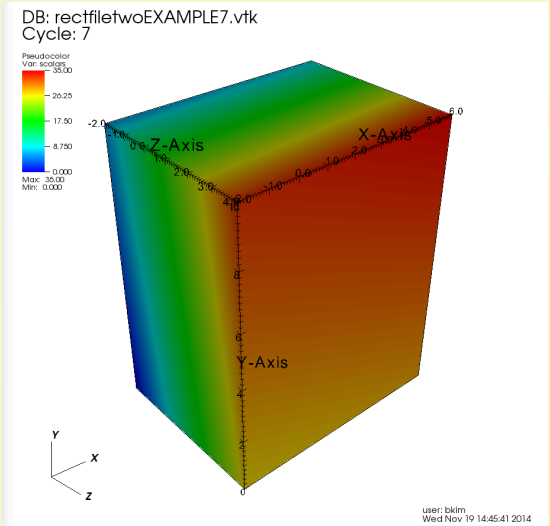












Try It

Visit Data Files:

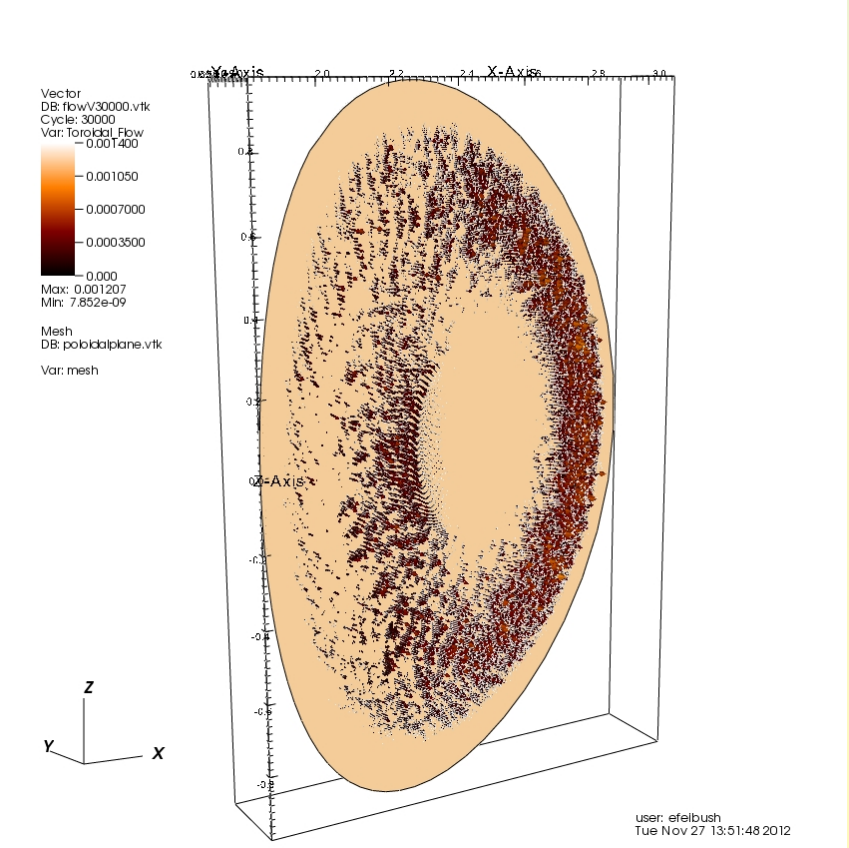
/Volumes/dll_drive/ViSIT DATA

Open File:

poloidalplane.vtk

Add Mesh→mesh

Attributes



Open File

flowV*.vtk database *

Add Vector→Toroidal_Flow

* “Smart” File grouping

(Turn off Grouping to load 1 file)

Time Step Movie - Demonstration

File → Save Movie

New Simple Movie

QuickTime

→

6 Frames per second

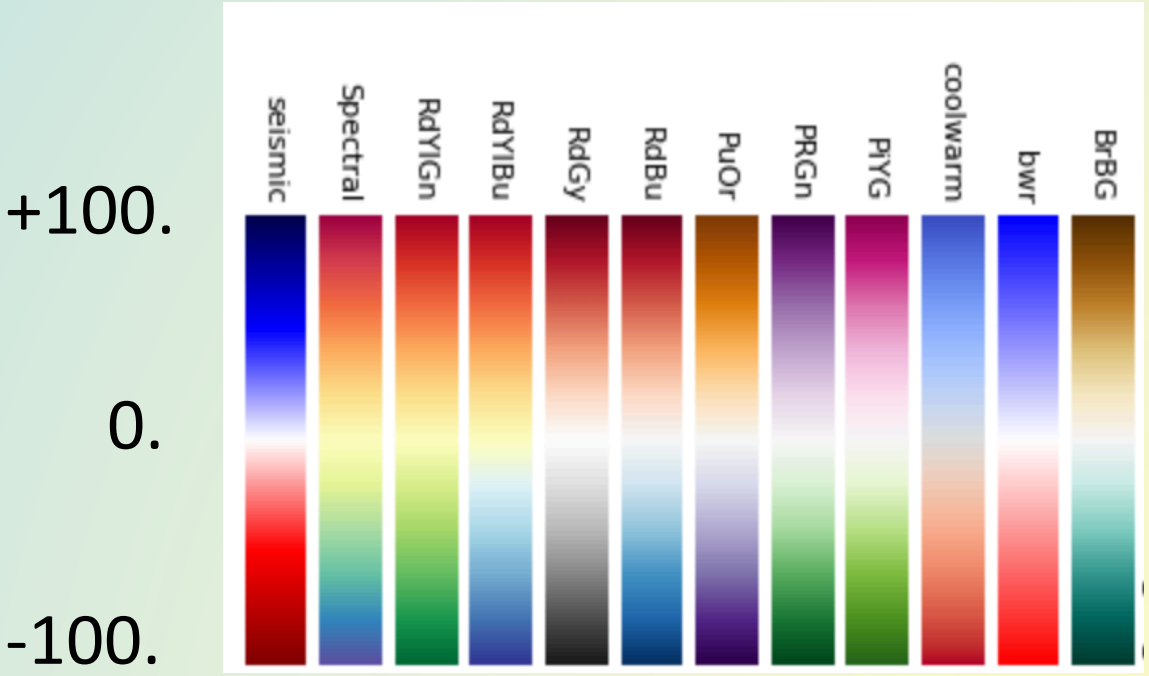
Click the arrow to apply your config

mpeg2encode in VisIt software distribution

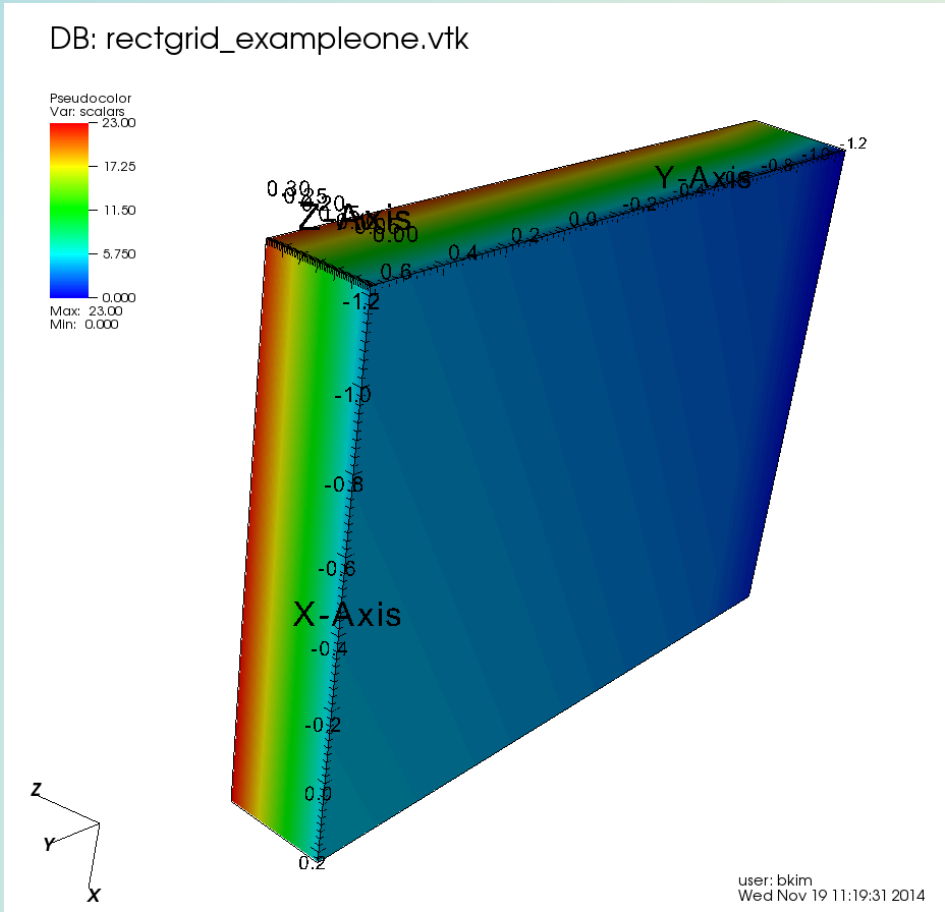
`mpeg1 format only`

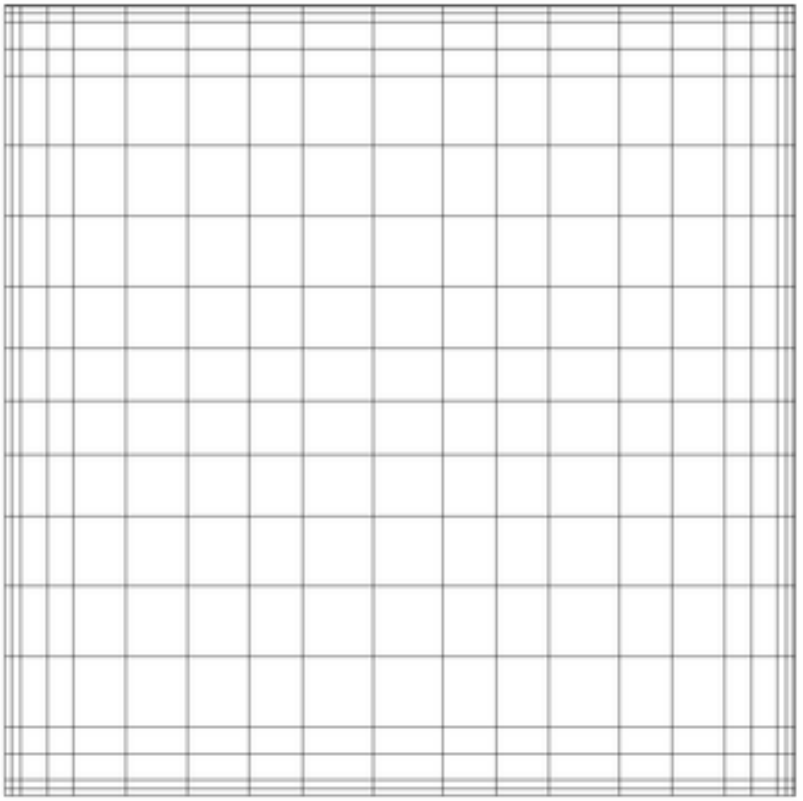
Color Maps

Divergent color maps



Rectilinear Grids

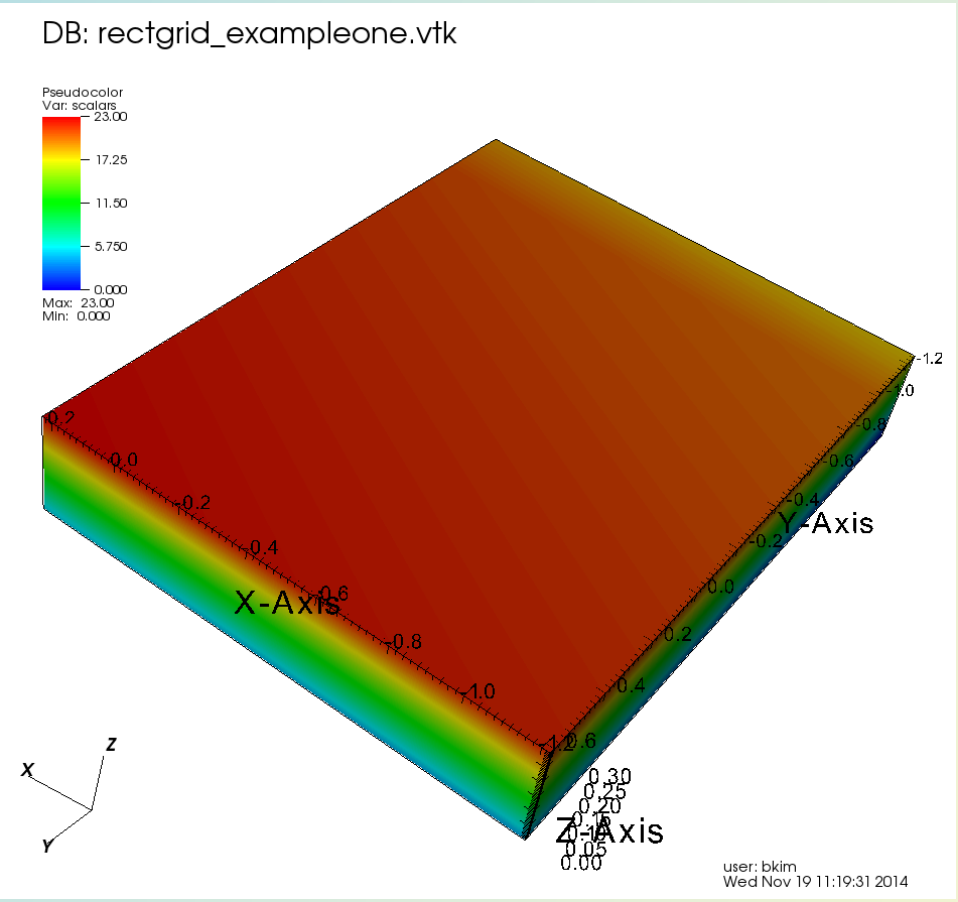




Continuous volume of data defined at specific points.

Non-Uniform spacing per axis.

Rectilinear Grids

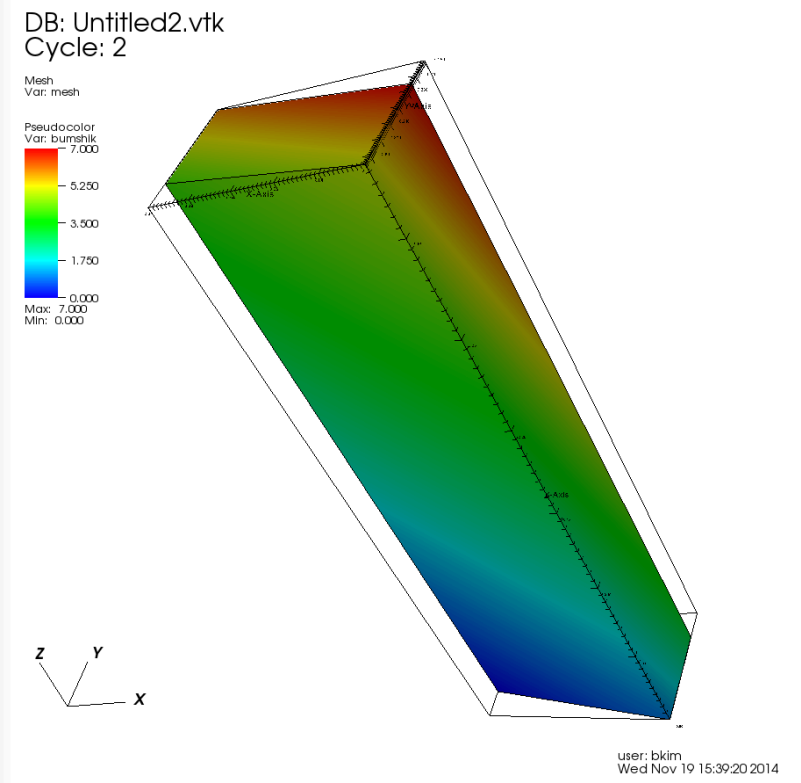


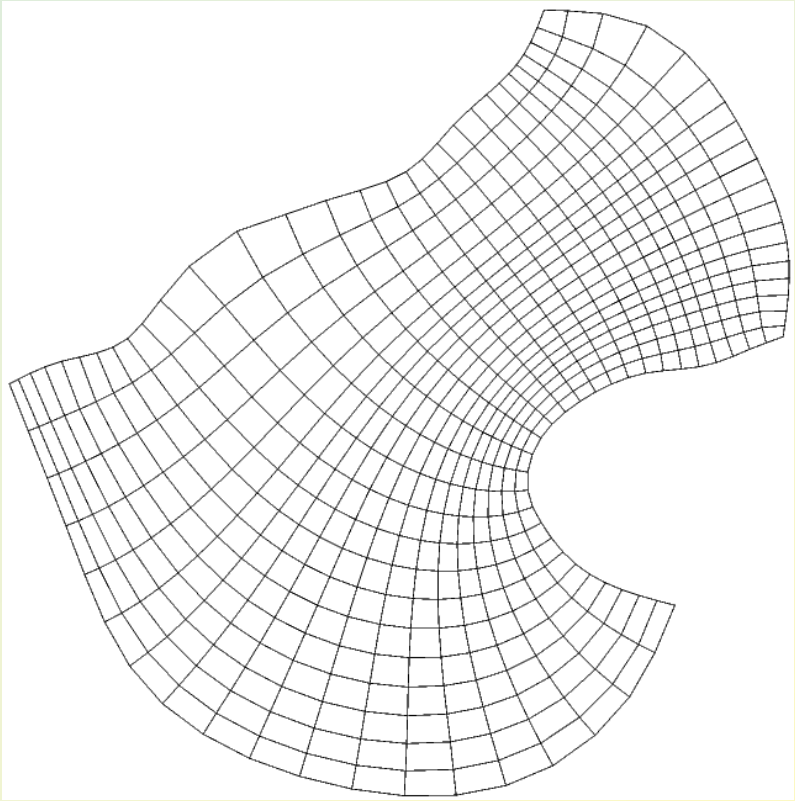
rectgrid_exampleone

```
# vtk DataFile Version 3.0
VTK format
ASCII
DATASET RECTILINEAR_GRID
DIMENSIONS 2 3 4
X_COORDINATES 2 float
-1.22 0.23
Y_COORDINATES 3 float
-1.25 -1.01 0.6125
Z_COORDINATES 4 float
0 0.1 0.2 0.3
POINT_DATA 24
SCALARS scalars float
LOOKUP_TABLE default
0 1 2 3 4 5 6 7 8 9 10
11 12 13 14 15 16 17 18 19
20 21 22 23
```

Non-Uniform Axis Spacing

Structured Grids





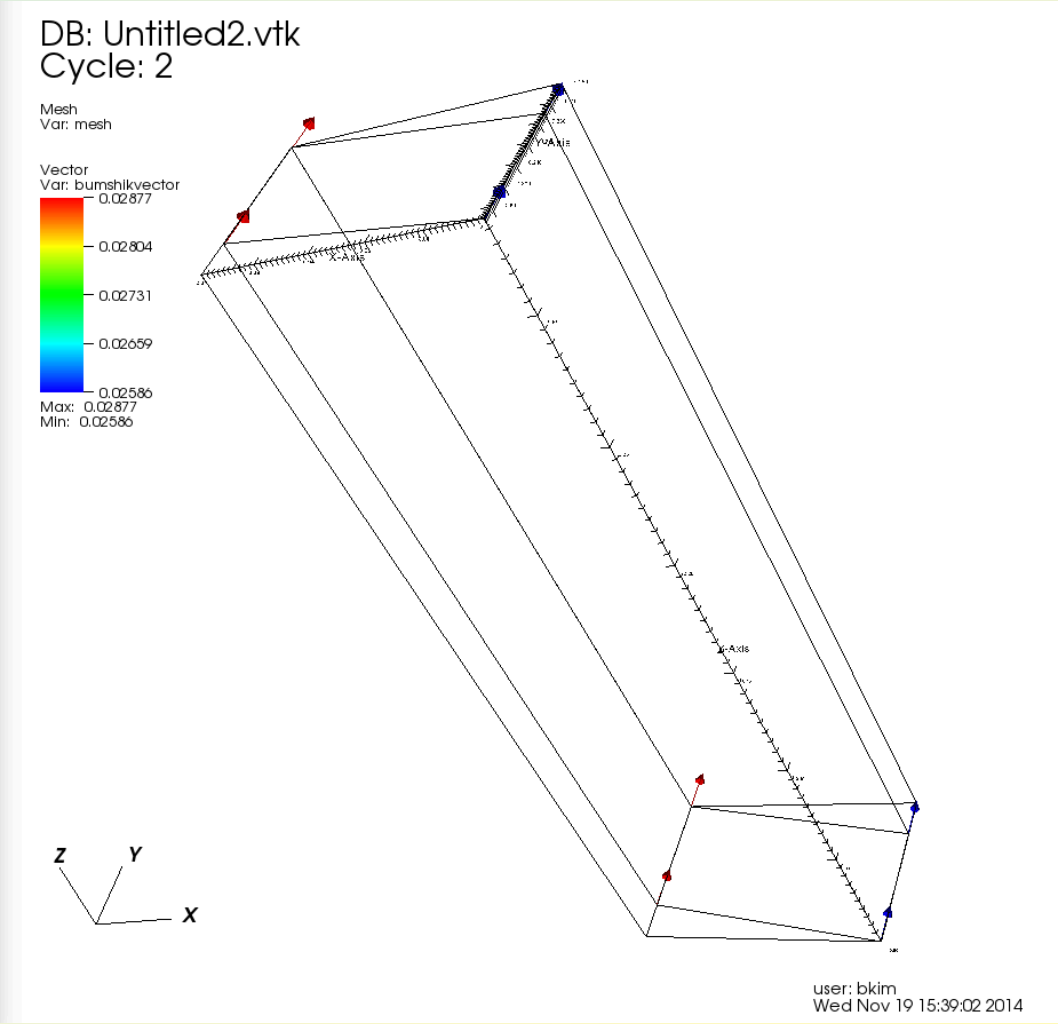
Continuous volume (or surface) of data defined at specific points.

Non-Uniform, Non-Orthogonal, any spacing per axis.
Quadrilateral cell faces. Can be curvilinear.

Structured Grids + Vectors

Untitled2.vtk

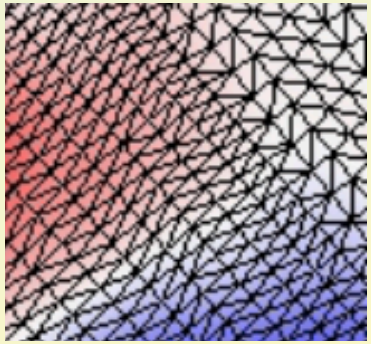
```
# vtk DataFile Version 3.0
vtk output
ASCII
DATASET STRUCTURED_GRID
DIMENSIONS 2 2 2
POINTS 8 float
0 0.2 0 0.1 0.184843 0 0 0.25 0
0.1 0.234843 0 0 0.2 0.333333 0.1 0.184843 0.333333
0 0.25 0.333333 0.1 0.234843 0.333333

POINT_DATA 8
SCALARS bumshik float
LOOKUP_TABLE default
0 1 2 3 4 5 6 7
VECTORS bumshikvector float
0 0.0287671 0 0 0.0258604 0 0 0.0287671 0
0 0.0258604 0 0 0.0287671 0 0 0.0258604 0
0 0.0287671 0 0 0.0258604 0
```



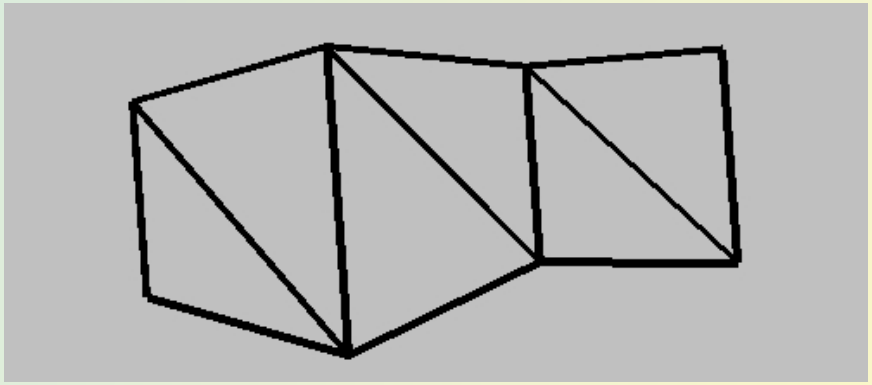
Grid Summary

Structured Points – uniform spacing, orthogonal
Rectilinear Grid – non-uniform spacing, orthogonal
Structured Grid – non-orthogonal quads

Unstructured Grid – any combination of polygons:



Triangle Strip

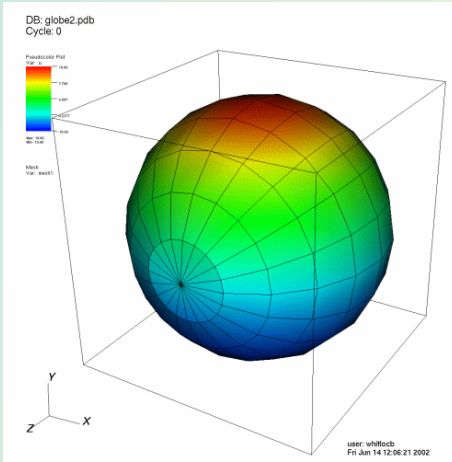


Paraview wiki: Users Guide VTK_Data_Model

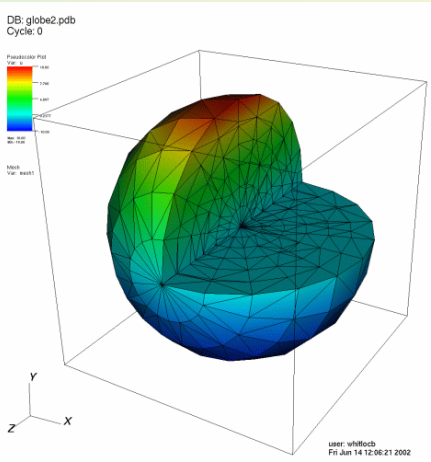
Geometric Selection - Clip Operator

- The Clip operator clips 2D or 3D plots against planes or a sphere to remove sections of the plots
- Use this operator when you want to see a cross section of a 3D plot, while still leaving the plot in 3D

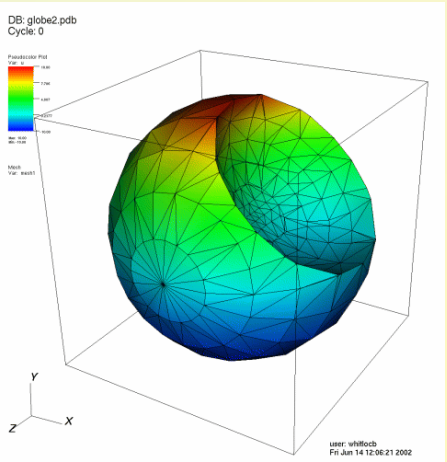
Original plots



Plots clipped with 2 planes



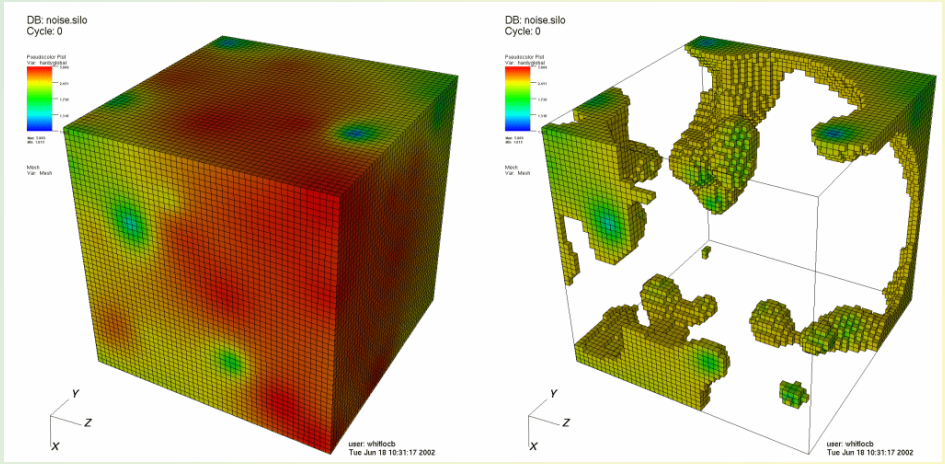
Plots clipped with a sphere



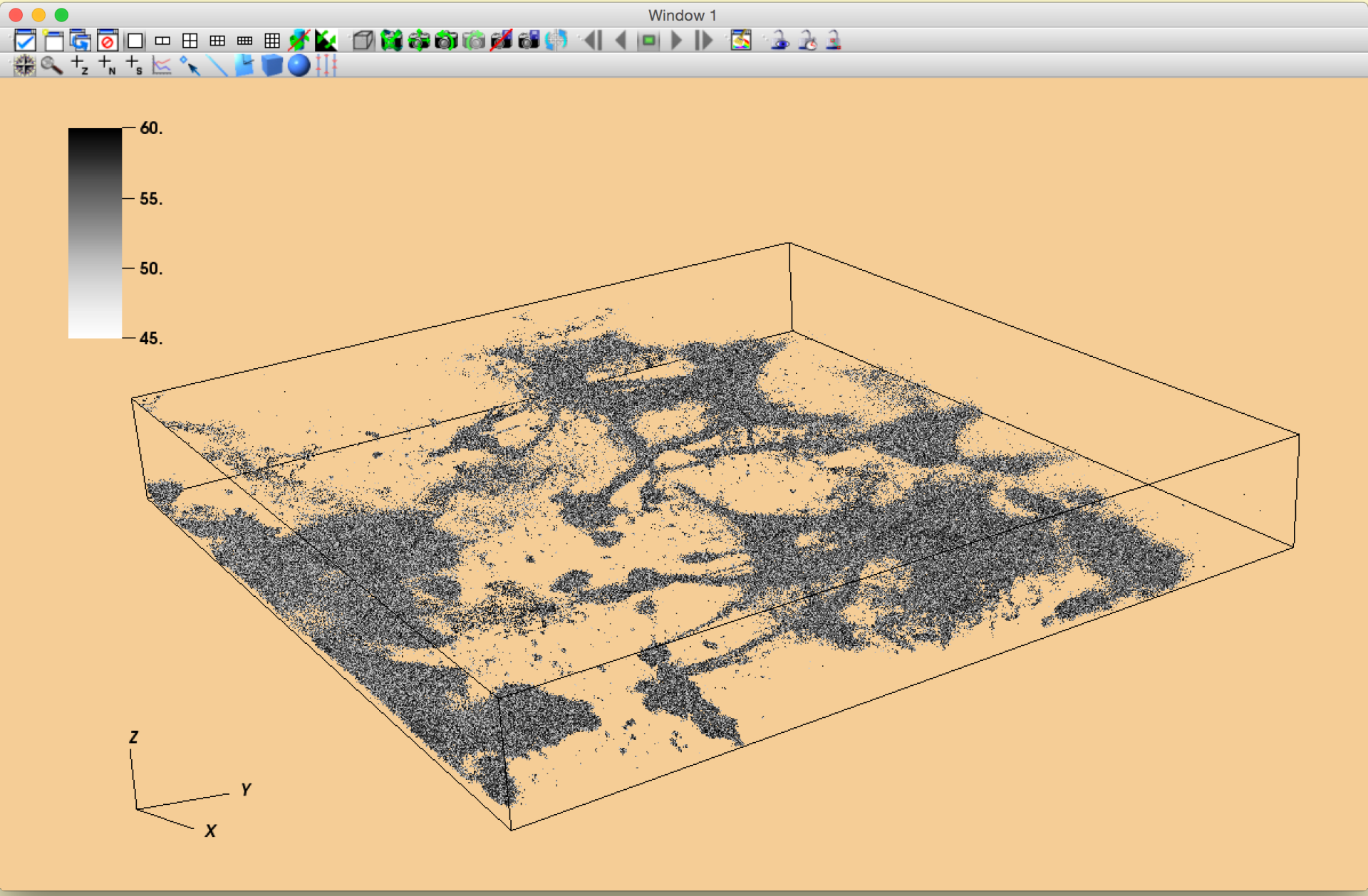
Data Value Selection - Threshold Operator

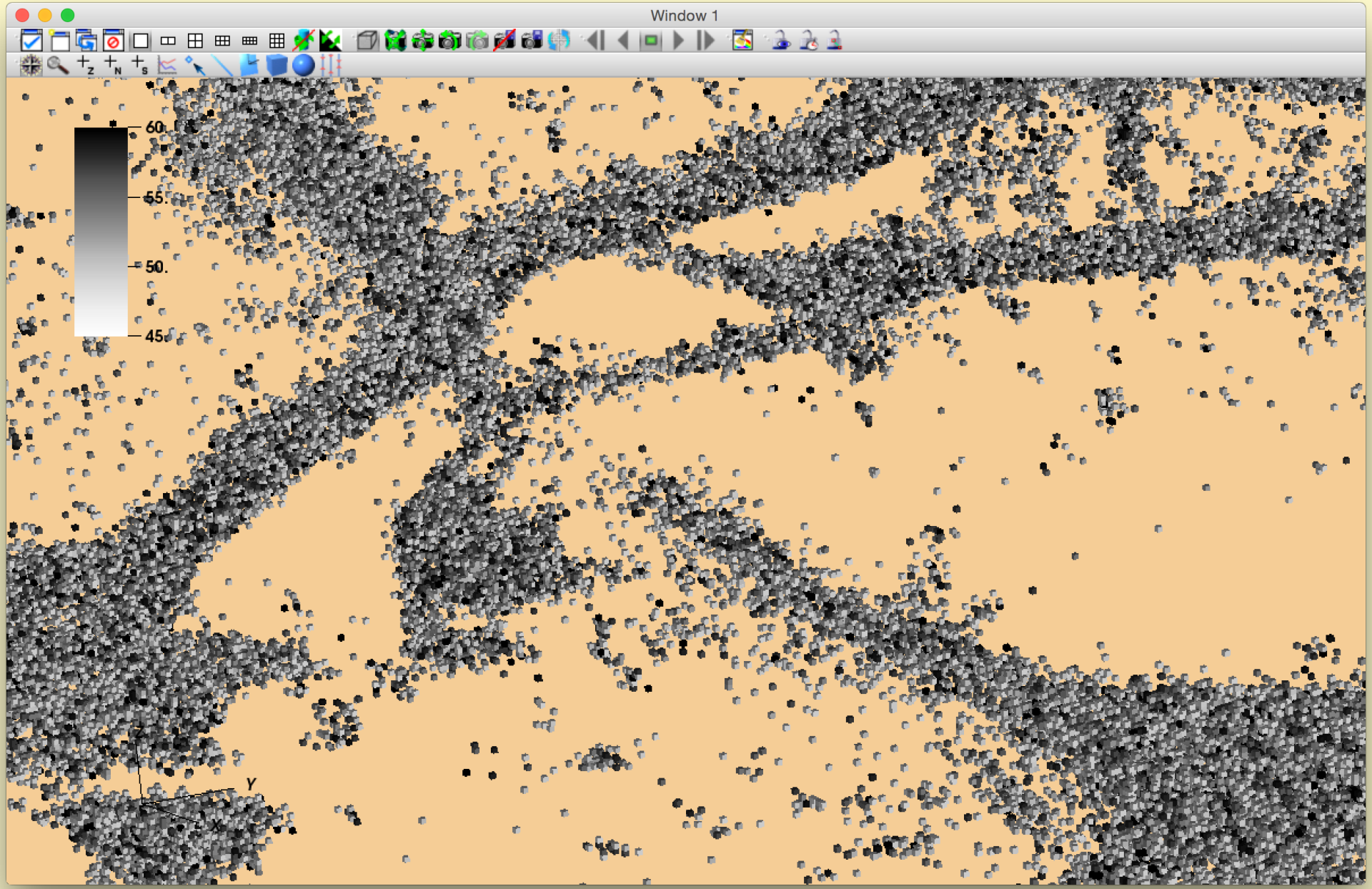
Use this operator to look only at cells that have values within a numerical range.

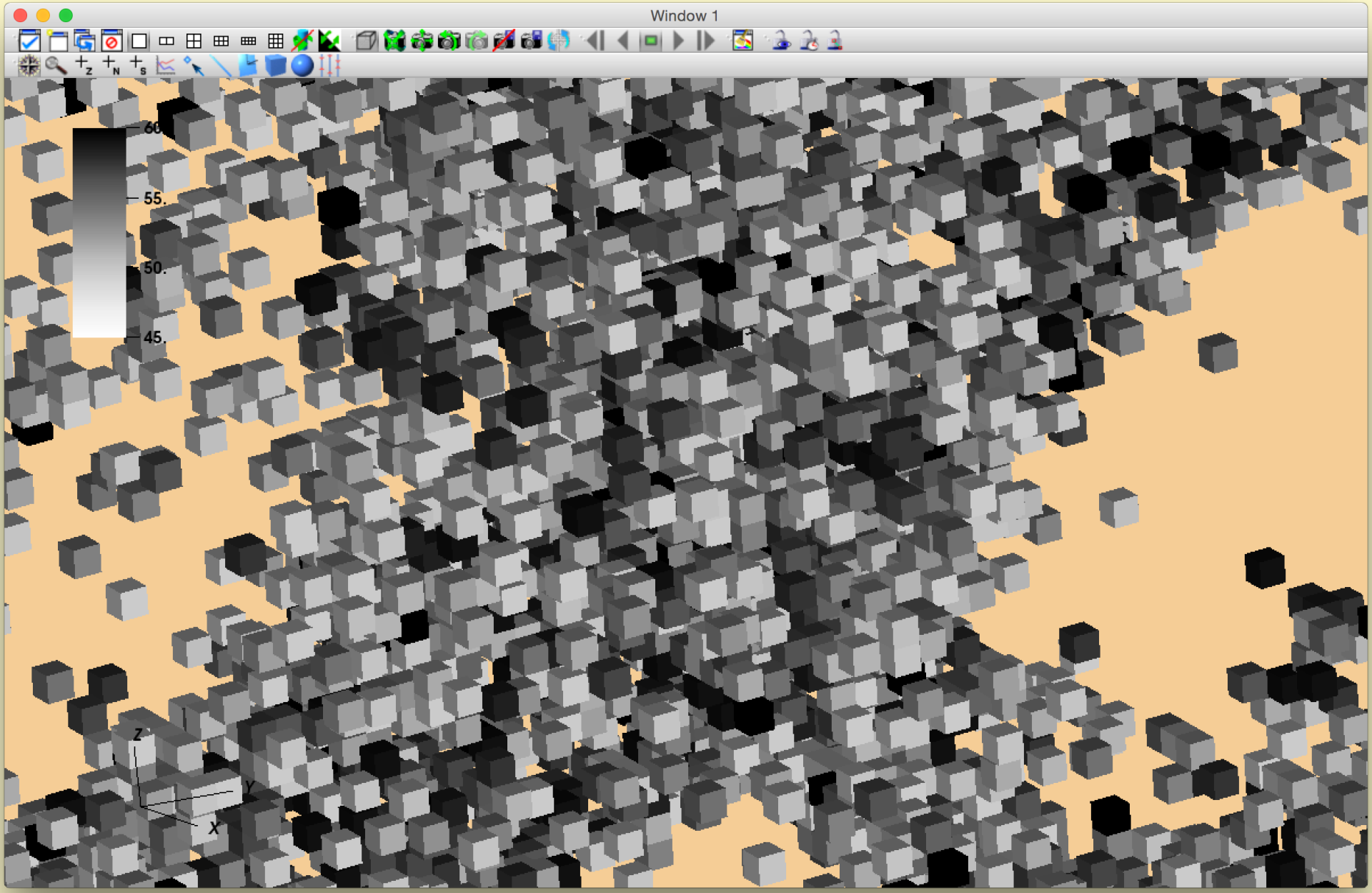
Removes cells whose value is not in the specified range.



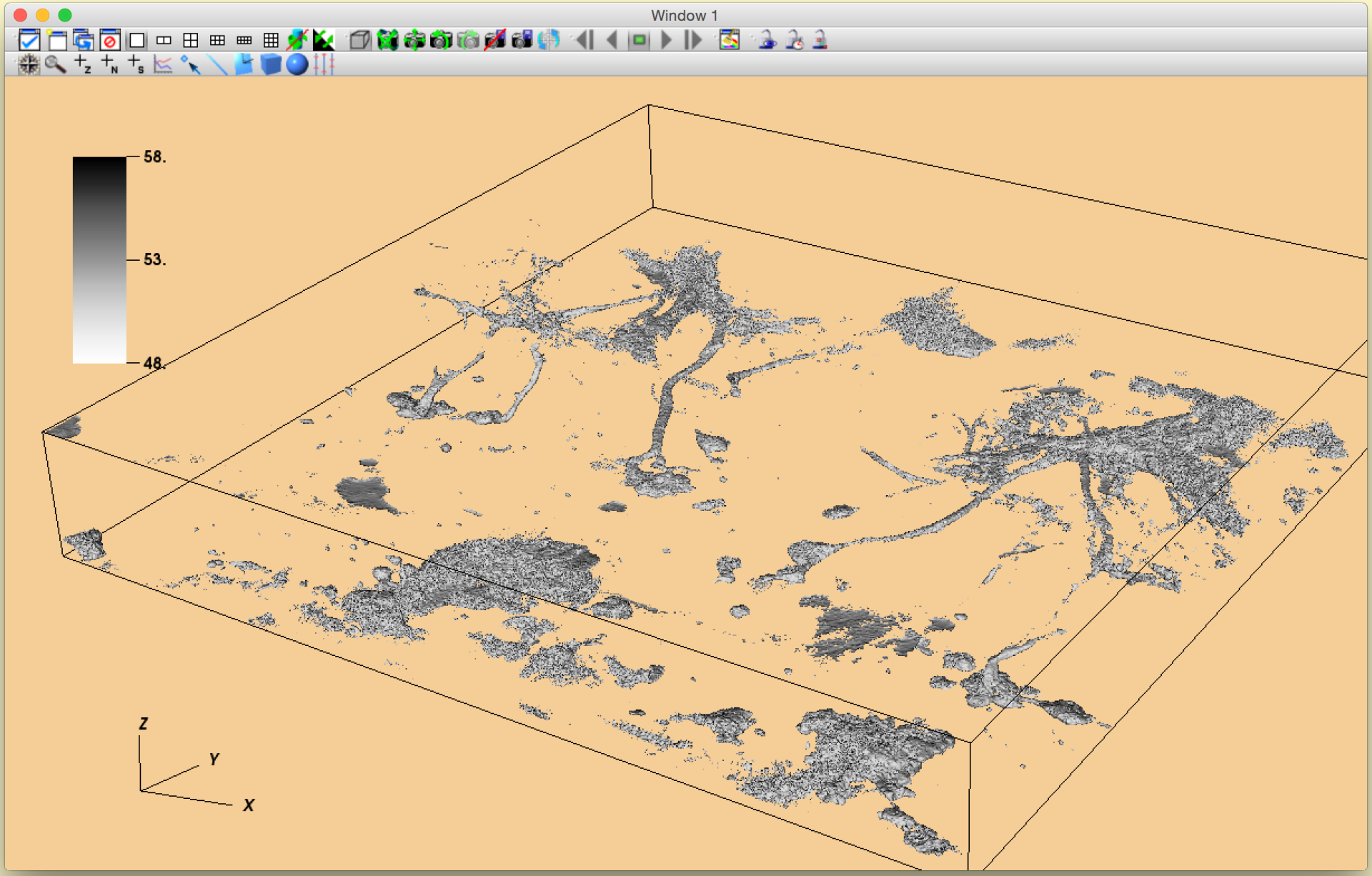
Threshold Operator

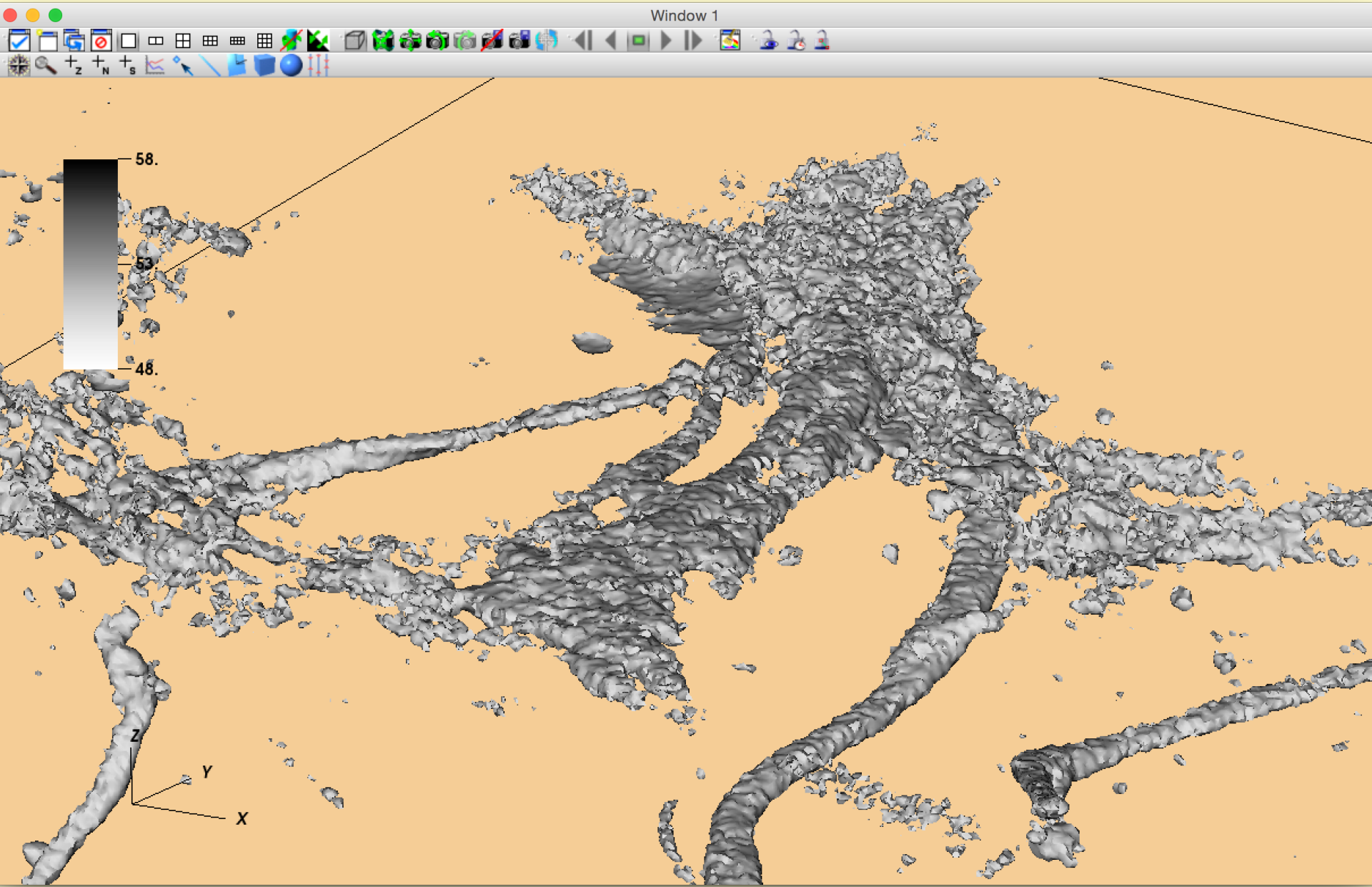



Window 1
60.
55.
50.
45.
Y
X


Window 1
60.
55.
50.
45.
Z
Y
X

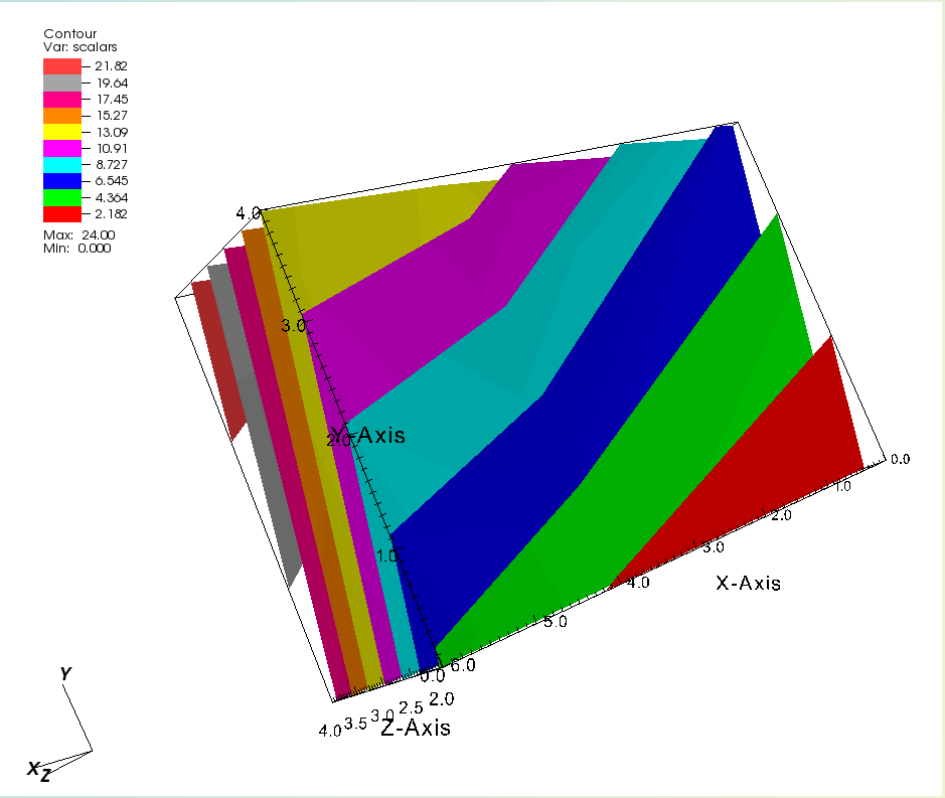
Isovolume Operator

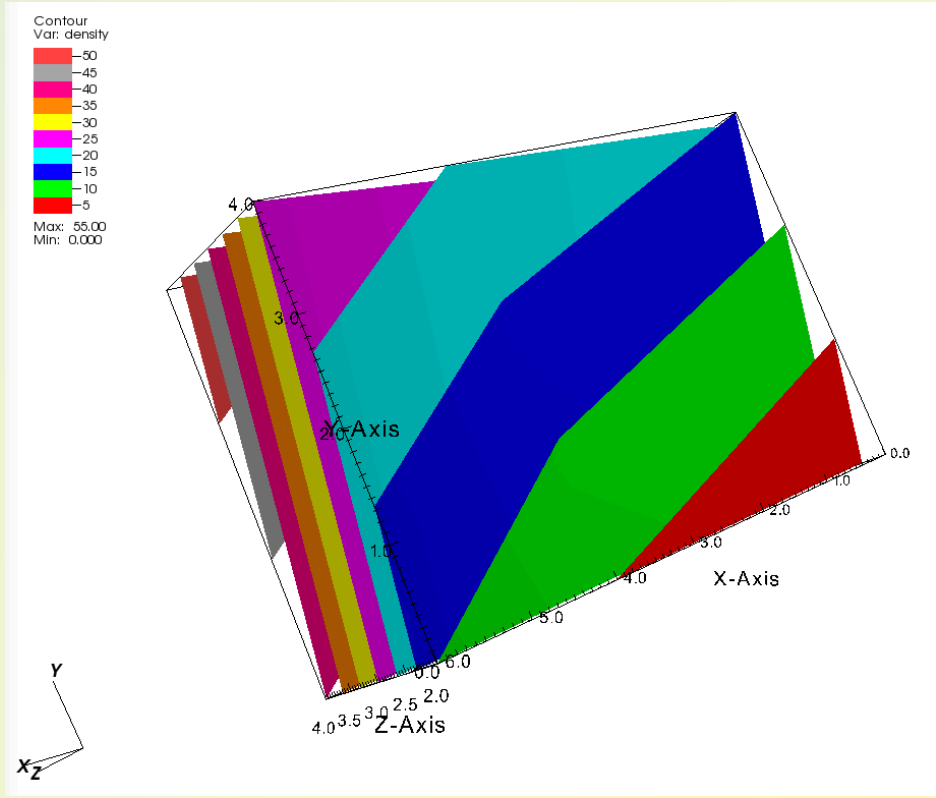


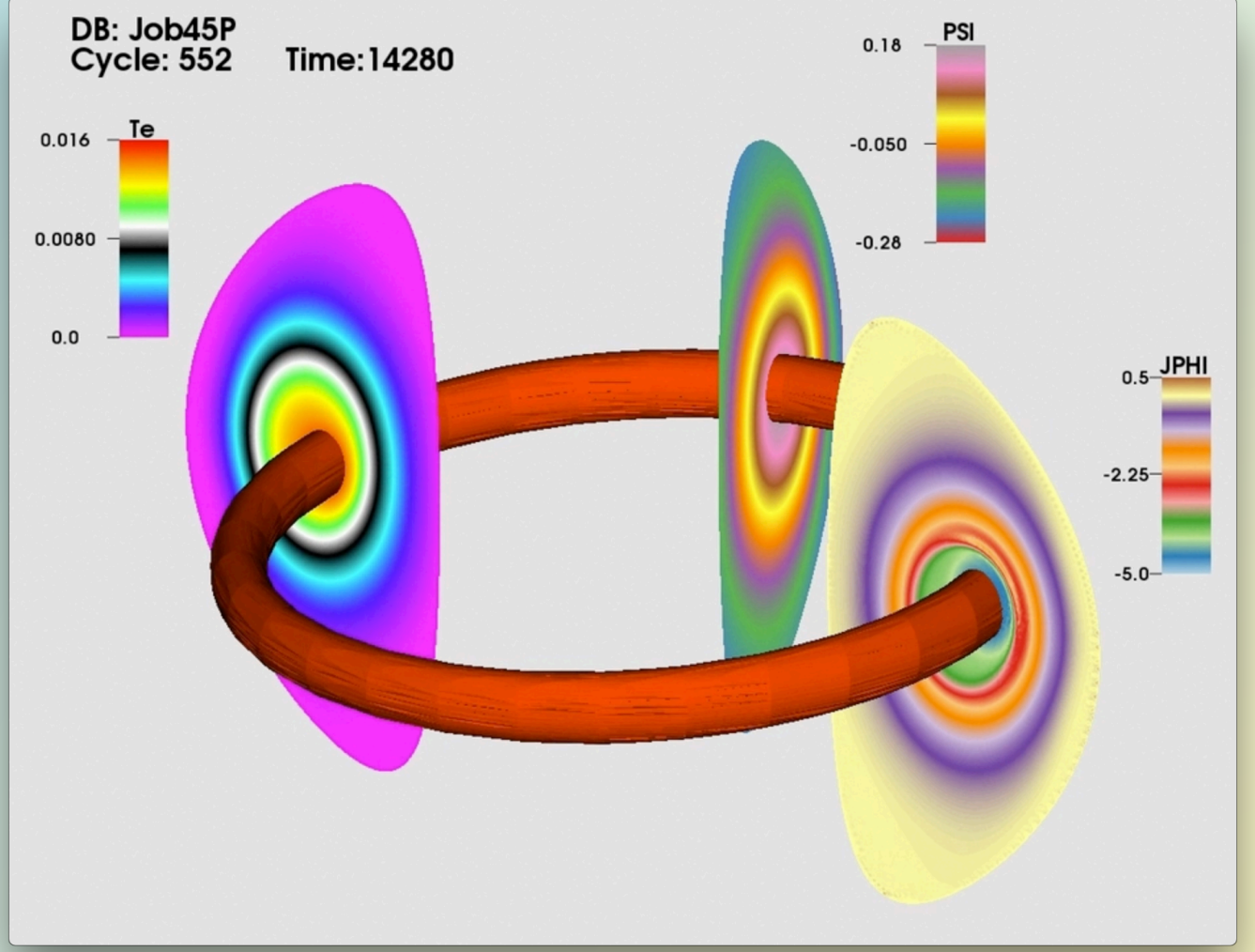

Window 1
58.
53.
48.
Z
Y
X

Data Value Selection – Isosurface Operator

Series of isosurfaces between data min-max.







Isosurface of Te = 0.015 at each time step.
Shows Te, PSI, and JPHI concurrently.

http://w3.pppl.gov/~efeibush/movies

teiso015.mov

Discrete Point Data

Define and display data at specific points in 3D.

Each point is a unique, independent sample.

Taken from compute grid (perhaps).

Look at data file:

```
x y z density
2.5  0.5  -0.1  .003
...
```

Polygons vs. Grid

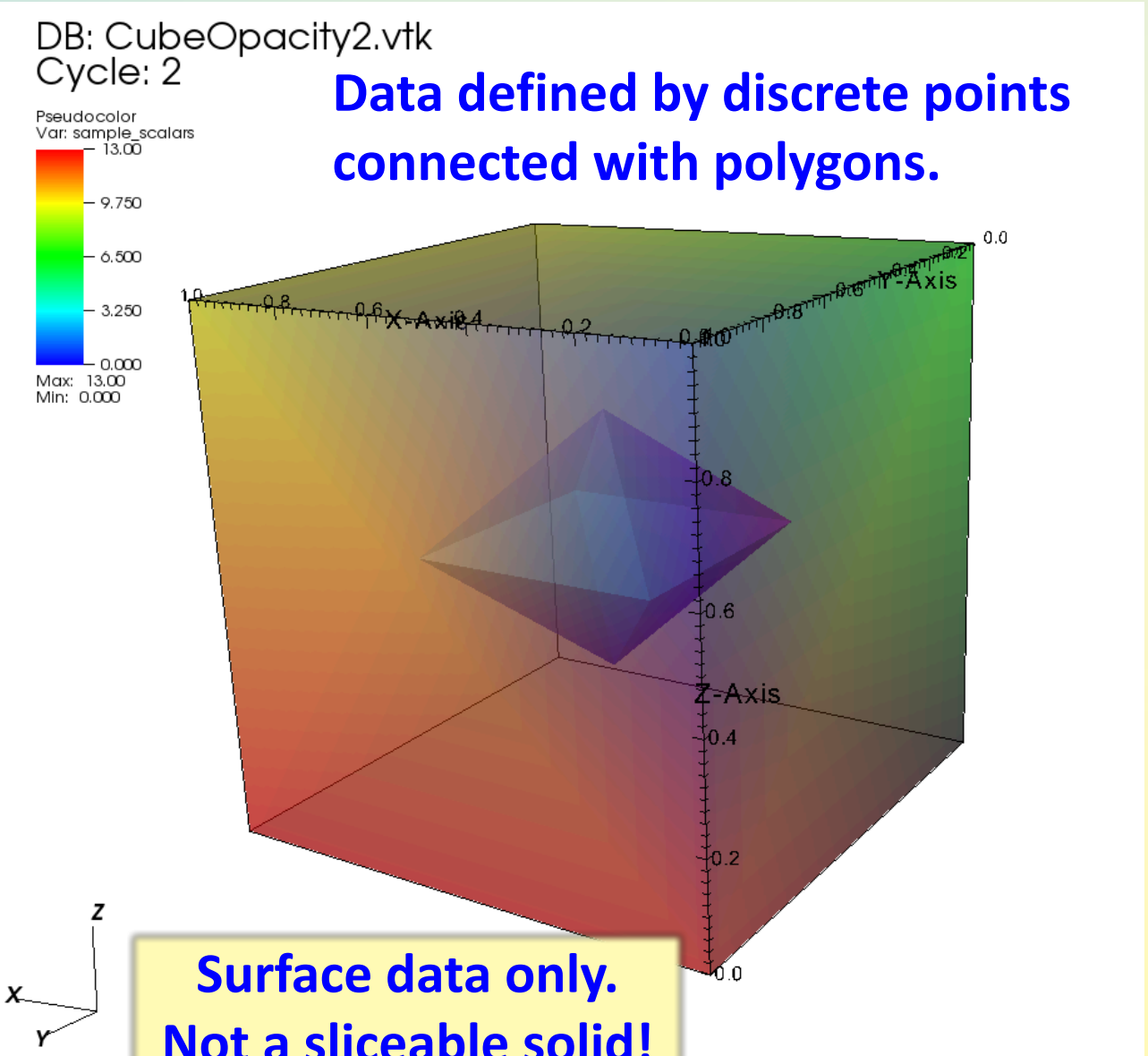
CubeOpacity2

```
# vtk DataFile Version 2.0
Cube example
ASCII
DATASET POLYDATA
POINTS 14 float
0.0 0.0 0.0
1.0 0.0 0.0
1.0 1.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
1.0 0.0 1.0
1.0 1.0 1.0
0.0 1.0 1.0
0.5 0.5 0.25
0.25 0.25 0.5
0.25 0.75 0.5
0.75 0.25 0.5
0.75 0.75 0.5
0.5 0.5 0.75

POLYGONS 14 62
4 0 1 2 3
4 4 5 6 7
4 0 1 5 4
4 2 3 7 6
4 0 4 7 3
4 1 2 6 5
3 8 9 10
3 8 9 11
3 8 10 12
3 8 11 12
3 11 12 13
3 9 11 13
3 10 12 13
3 9 10 13

POINT_DATA 14
SCALARS sample_scalars float 1
LOOKUP_TABLE my_table
 0.0
 1.0
 2.0
 3.0
 4.0
 5.0
 6.0
 7.0
8 9 10 11 12 13
```

POINTS

POLYGONS

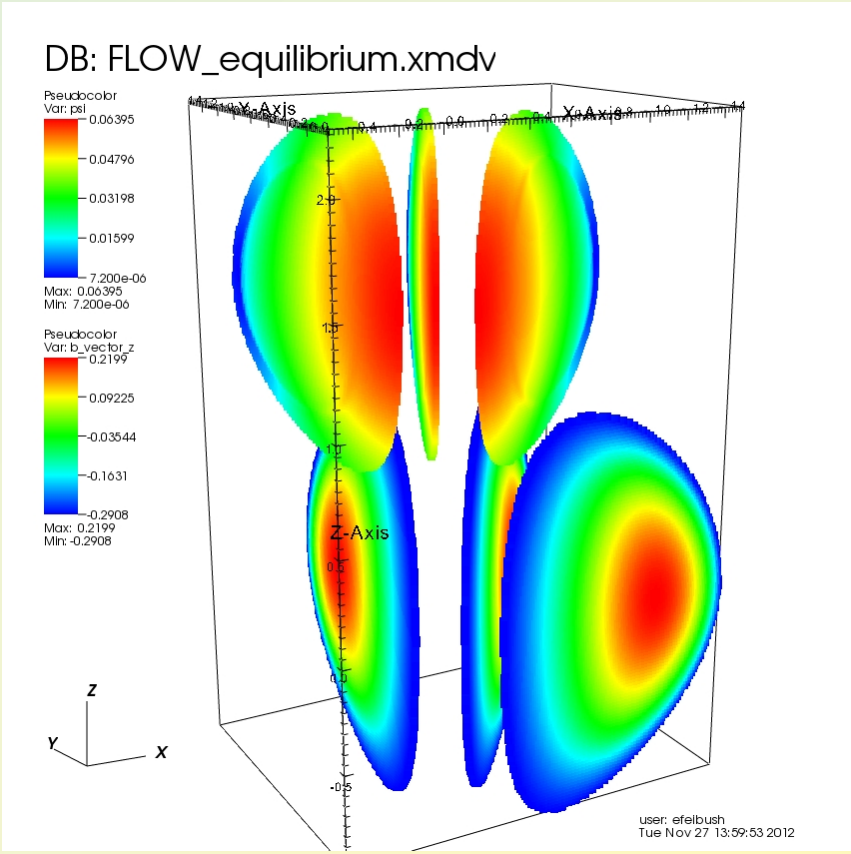
VALUES



Transforms

Relocate geometry

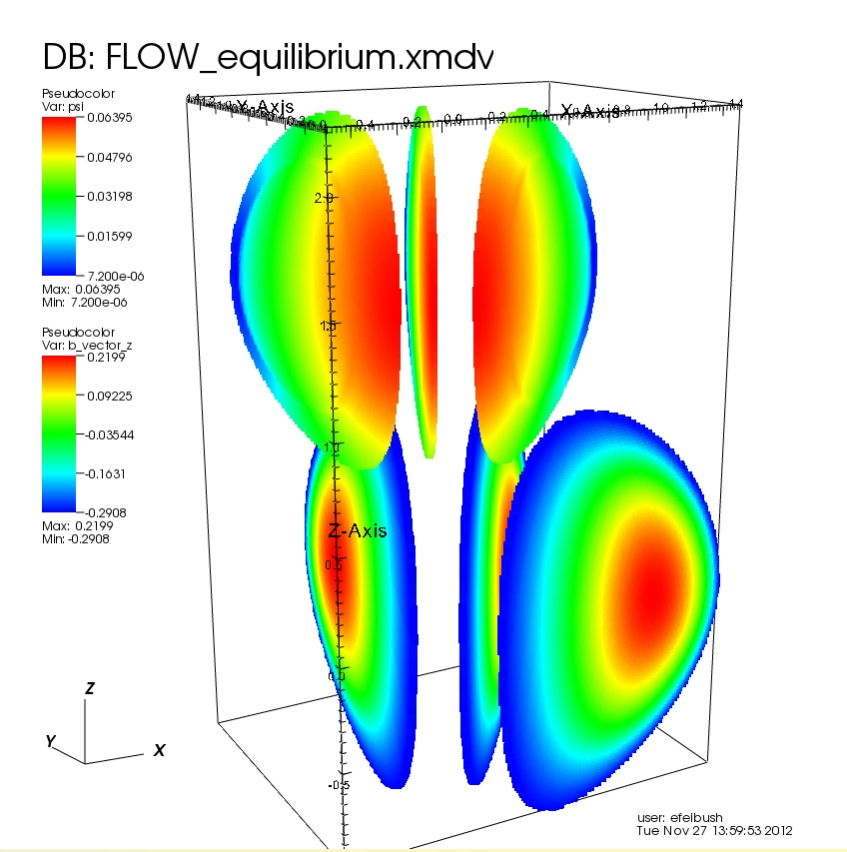
- Translate
- Rotate
- Scale



Try It

Open File

FLOW_equilibrium.xmdv



Add Pseudocolor→psi

Turn off Apply operators to all plots

Add Pseudocolor→b_vector_z

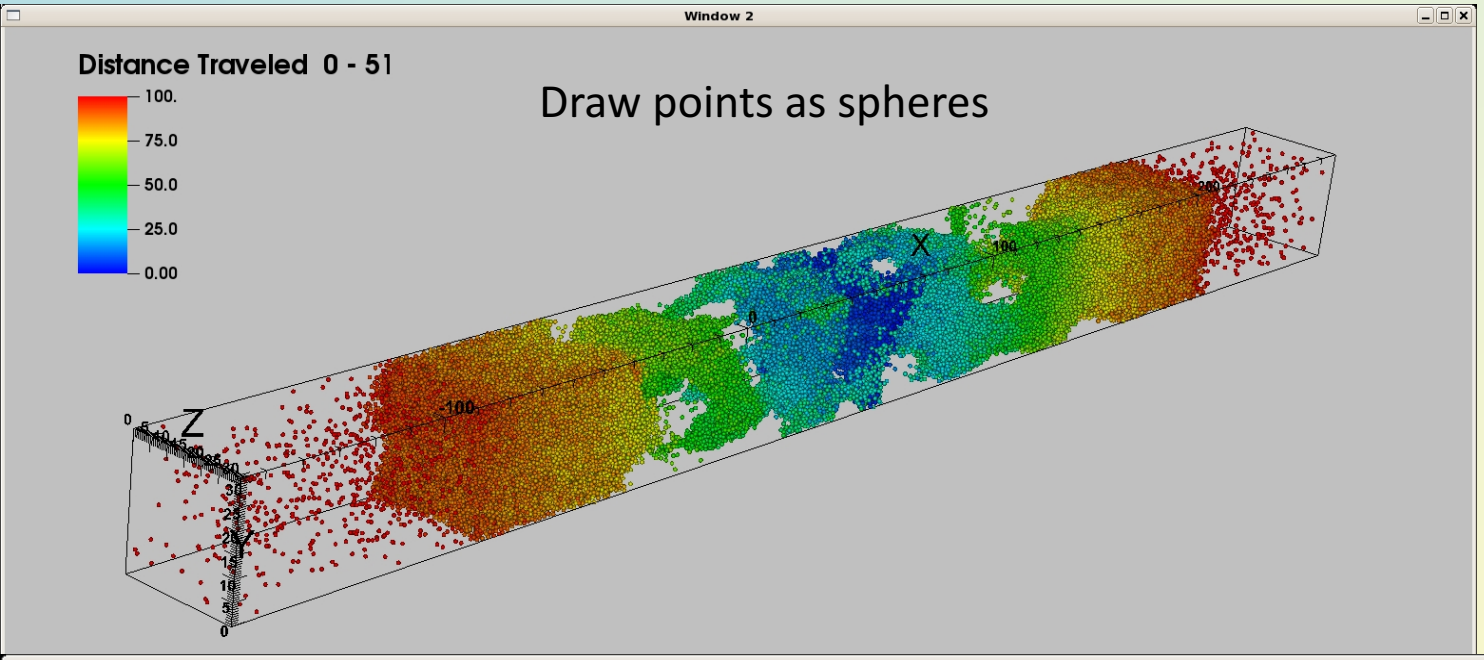
Operators→Transforms→Transform

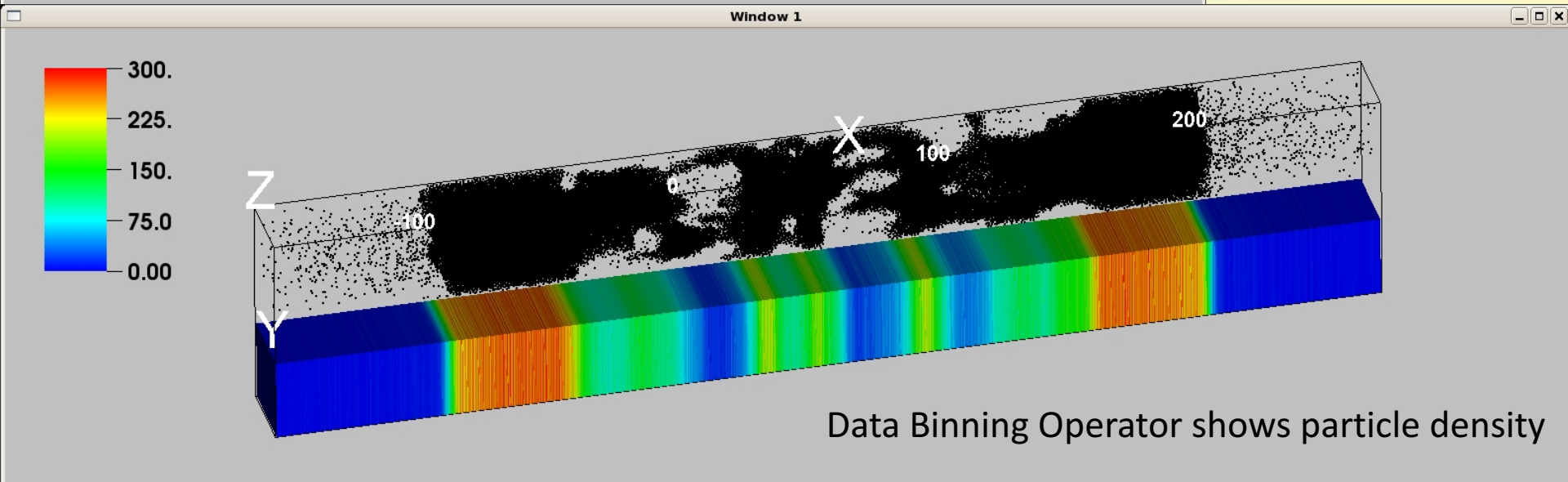
Rotate 25 degrees

Translate Z 1.5

xmdv – multiple scalar variables per point

Molecular Dynamics Example





Data Binning Operator shows particle density

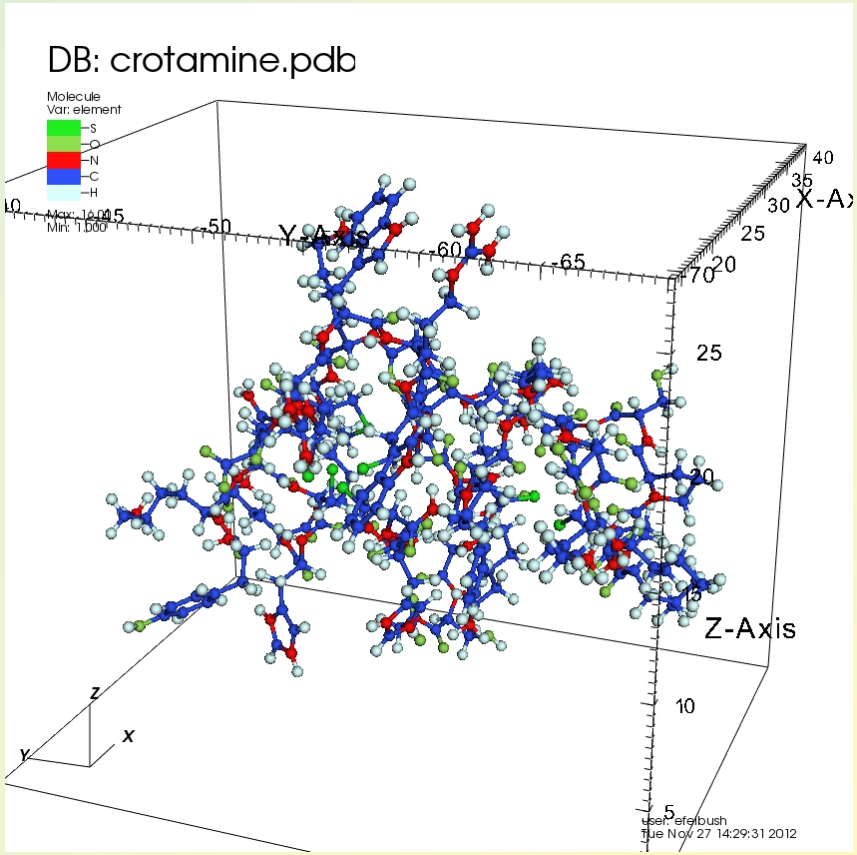
Try It

Open File crotamine.pdb

(Protein Data Bank)

Add Molecule→element

attributes



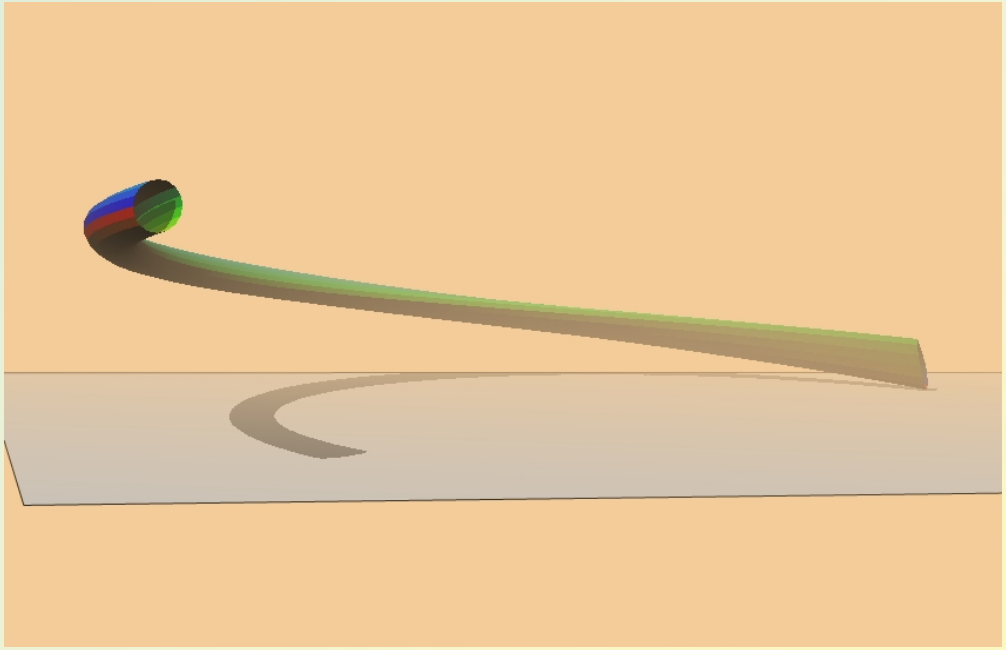
Try It

Open File base.vtk

Open File fluxtube.vtk

Options→Rendering ...

Controls→Lighting



Animation

Time step
Variable index
Geometry change

View
    Operators (slice, clip, etc.)

Simple VTK file time steps
        or
Complex python scripting

jpeg, png files → QuickTime .mov

    Python interpreter -

```
import myscript
   [ edit, retry ]
reload(myscript)
```

Movie Maker Program (1)

- Java – portable to Linux, Mac, Windows
  - Based on Sun's javax.media package.
- Reads all images in directory – JPEG, PNG
  - ImageMagick: mogrify -resize 100% *.jpeg
- Creates QuickTime movie file - .MOV

princeton.edu/~efeibush/makemovie

`iJpegImagesToMovie.jar`

Movie Maker Program (2)

ffmpeg

- Most comprehensive
- Command line Linux
- tigressdata

- Downloads for Mac & Windows

- mpeg2encode in VisIt software installation

Mac: Time Lapse Assembler → QuickTime .mov

Movie Maker Program (3)

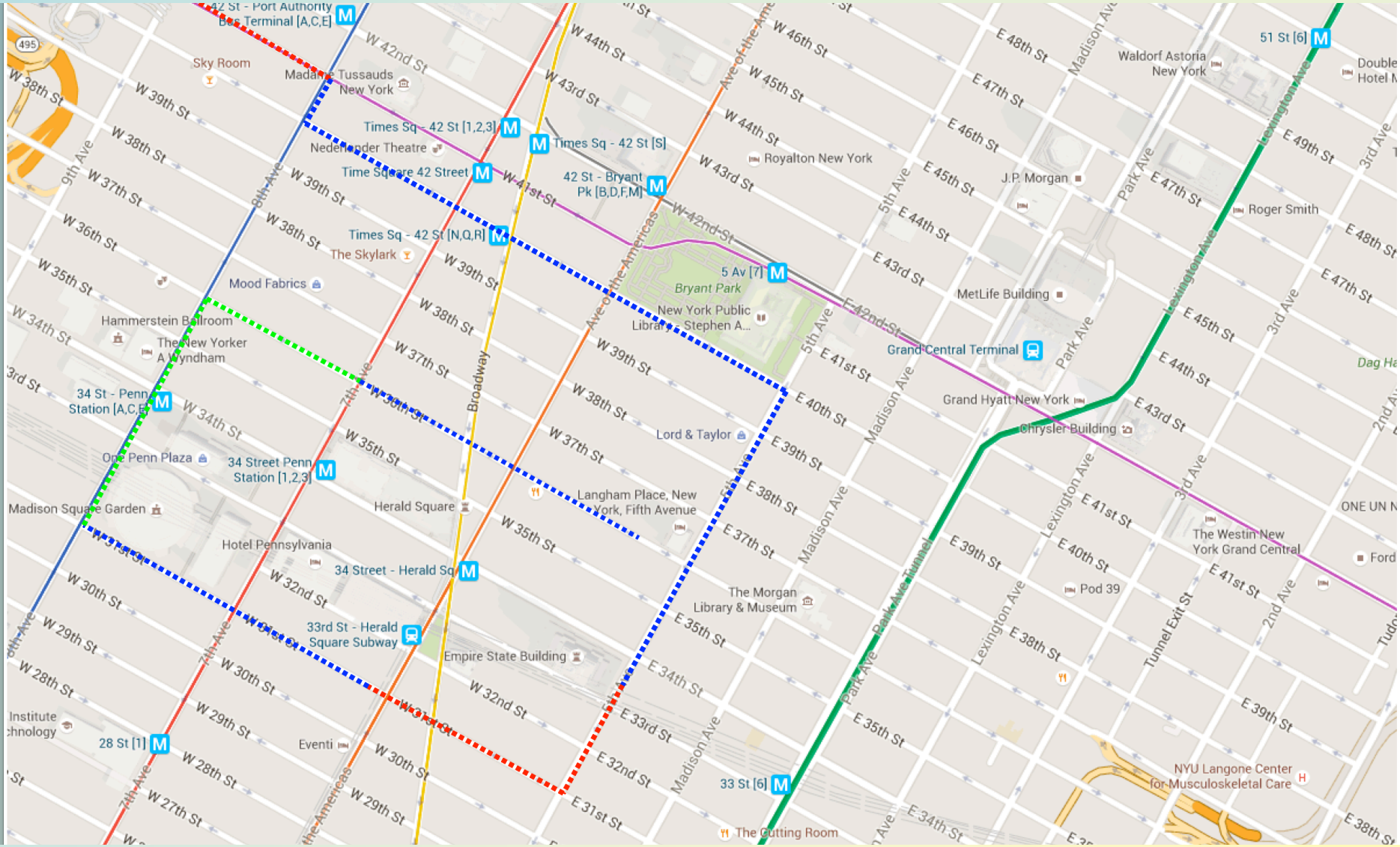
Titles - iMovie, Adobe Premier

Video

Audio

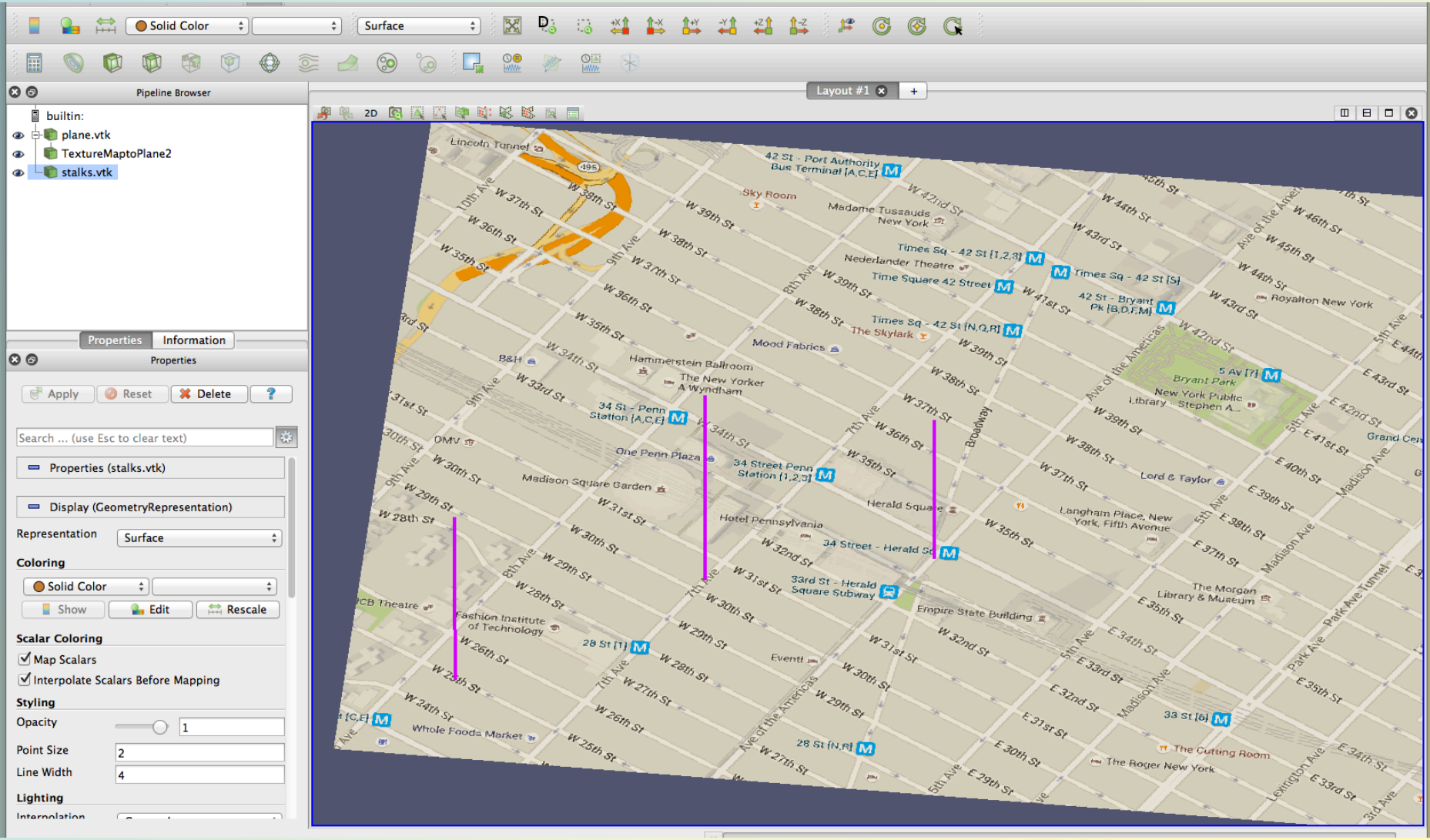
Digital Learning Lab resources

Geo-Locate with Maps



Paraview

Texture Rendering + VTK → 3D View



Summary of Today's Features

Plots + Attributes
- Mesh
- Pseudocolor
  - Points, Lines, Vectors, Polygons, Mesh – Color Tables
- Contour
- Molecule
- Volume

Data files
- VTK
- Point3D, xmdv

Transform operators
- Scale, Rotate, Translate

Selection operators
- Clip
- Box
- Threshold

Slicing operators
- Slice, ThreeSlice
- Isosurface

Viewing

Lighting, Shadow, Depth-Cue

Annotation

Animation
- Simple Time Slider movie
- Python scripting

Images to QuickTime movie

https://wci.llnl.gov/simulation/computer-codes/visit - Downloads

Just search for: "visit visualization"

visitusers.org search …

Getting Data Into VisIt - document (& your project)

VTK - text or binary

VTK File Formats - vtk.pdf on my website www.princeton.edu/~efeibush

Visualization with VisIt mini-course

paraview.org

Contact

Eliot Feibush

efeibush@princeton.edu

243-2695

www.princeton.edu/~efeibush/viscourse

Vis office hours: Thursday 2 pm Lewis 347

Tuesday afternoon possible

New Vis Lab: 4K screens = 16 million pixels on the wall.

Remote Vis at Princeton

Large amount of data on HPC tigress.

Display without copying data.

Render on tigressdata GPU instead of laptop.

Large Clusters	Processor Speed	Nodes	Cores per Node	Memory per Node	Total Cores	Inter-connect	Performance: Theoretical
TigerGPU **Dell Linux Cluster**	2.4 GHz Xeon Broadwell E5-2680 v4 1328 MHz P100 GPU	80	28 4 GPU/node	256 GB 16 GB/GPU	2240 320 GPUs	Omnipath	86 TFLOPS 1504 TFLOPS
TigerCPU **HPE Linux Cluster**	2.4 GHz Skylake.	408	40	192 GB (40 w/768 GB)	16320	Omnipath	>1103 TFLOPS
Della **Dell Linux Cluster**	2.5 GHz_Ivybridge 2.6 GHz_Haswell 2.4 GHz_Broadwell 2.4 GHz_Skylake	80 32 48 64	20 20 28 32	128 GB 128 GB 128 GB 192 GB	5632	QDR Infiniband	267+ TFLOPS
Perseus **Dell Linux Cluster**	2.4 GHz Xeon	320	28	128 GB	8960	FDR Infiniband	344 TFLOPS

Smaller Systems	Processor Speed	Nodes	Cores per Node	Memory per Node	Total Cores	Interconnect	Performance
Adroit **Dell Linux Cluster**	2.6 GHz Skylake 705 MHz K20	9 4	32 4 GPU/node	384 GB 5.0 GB/GPU	288	FDR Infiniband	3.2 TFLOPS 9.36 TFLOPS
Tigressdata **Dell Linux Server**	2.4 GHz Gold 6148 Xeon	1	40	768 GB	20	N/A	400+ GFLOPS
Nobel **Dell Linux Server**	2.3 GHz Haswell	2	28	224 GB	56	N/A	1.03 TFLOPS

Princeton Research Computing

Help Sessions
FAQs
Online Tutorials

FAQs

Introduction

- What is a cluster?
- What is /tigress?
- What is a GPU?

Miscellaneous

- Why can't I login to a cluster using SSH?
- How to word Acknowledgement for use of clusters/systems for Publication
- When do systems undergo scheduled maintenance
- How do I use VNC on tigressdata?
- How do I connect to one of the nobel machines directly?
- Using Filezilla with the nobel system
- Making Duo access more convenient

More Questions and Answers: AskRC

A collection of questions and answers contributed by Research Computing users and staff members can be found at AskRC.

ssh tigressdata

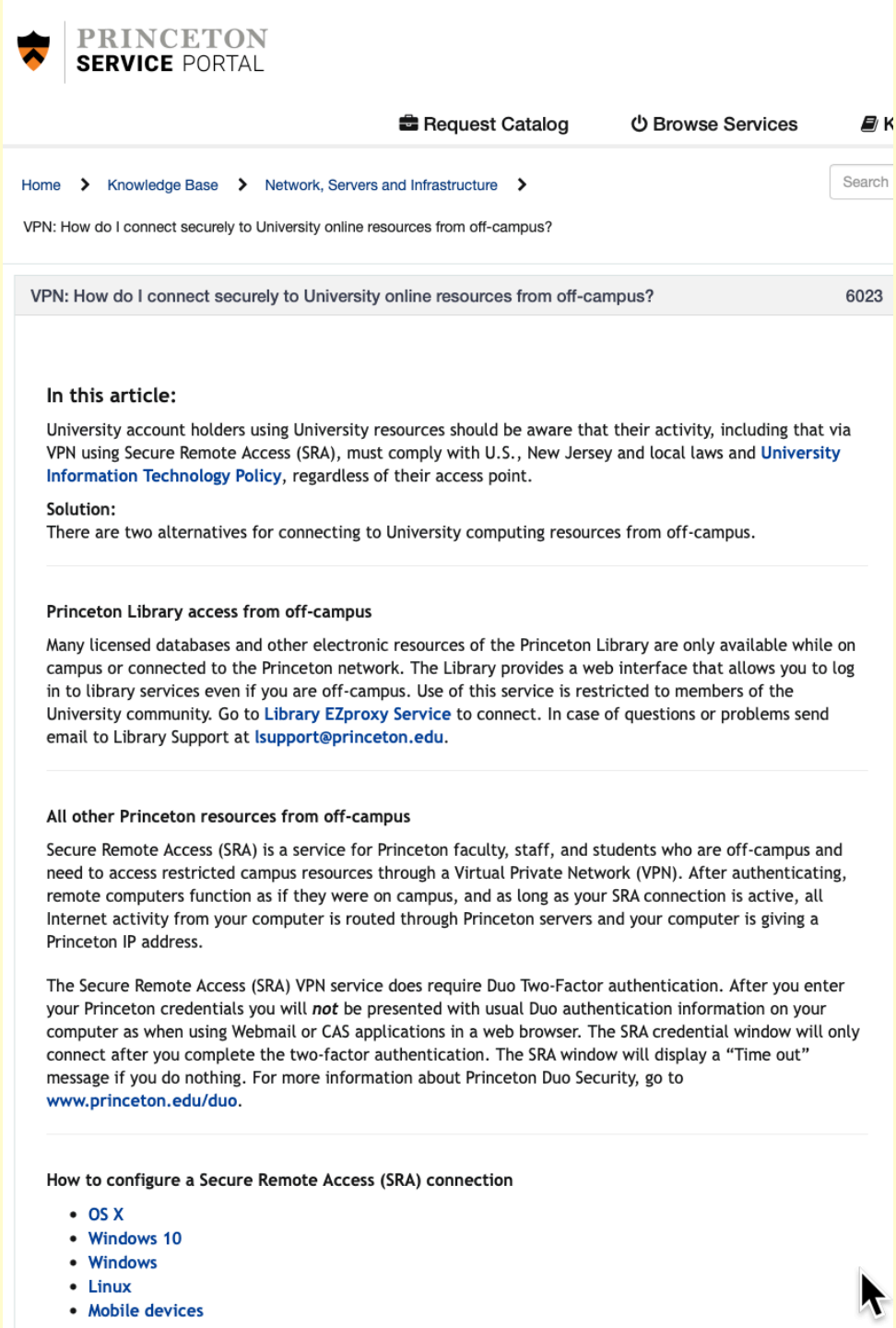
Off-Campus Considerations

How to ssh to tigressdata

VPN

OIT web page - search for VPN

How do I connect to University online resources from off-campus?

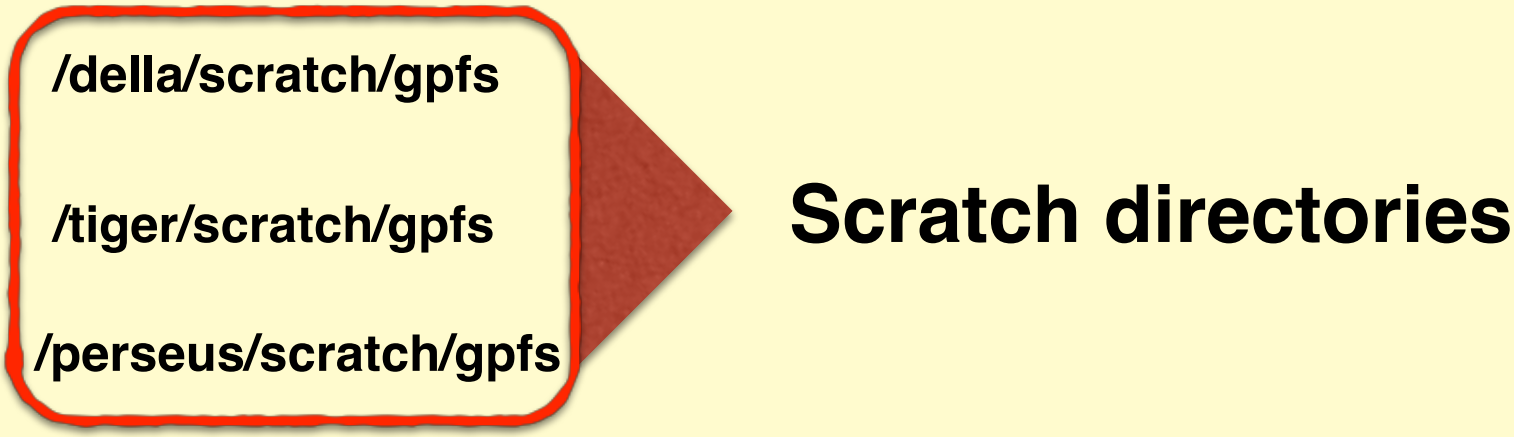


tigressdata.princeton.edu

File System

df command shows:

/tigress



tigressdata Remote Vis

TurboVNC remote desktop, Client - Server architecture

3 Step Process

1. Start vncserver on tigress data
2. Establish tunnel from your computer to tigress data
3. Run vncviewer on your computer (client)

search: turbovnc
Install from
sourceforge.net/projects/turbovnc

1. Start VNC Server

ssh tigressdata

$ module load turbovnc

$ vncserver

$ vncserver -list

note X Display # such as :2

First time: create password, stored in ~/.vnc/passwd ***(delete file to reset)***

2. Establish Tunnel
(because turbovnc is not encrypted)

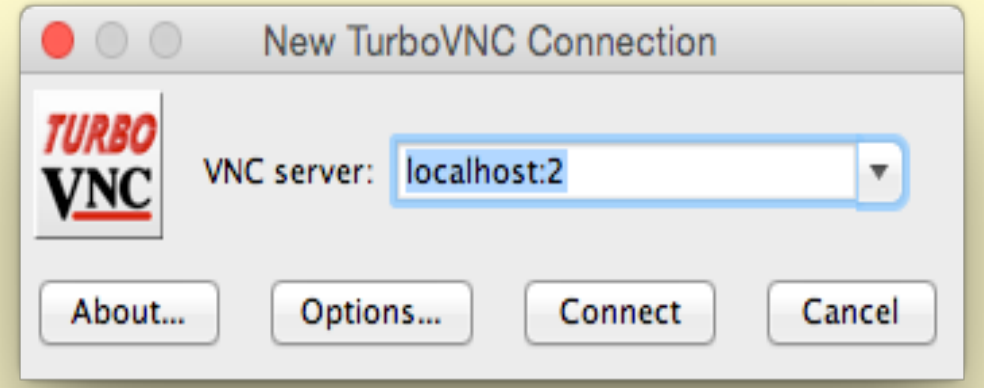
ssh -A -L 5902:localhost:5902 efeibush@tigressdata

5900 + X Display # ***(hence step 2 is after step 1)***

-A Enables authentication forwarding.

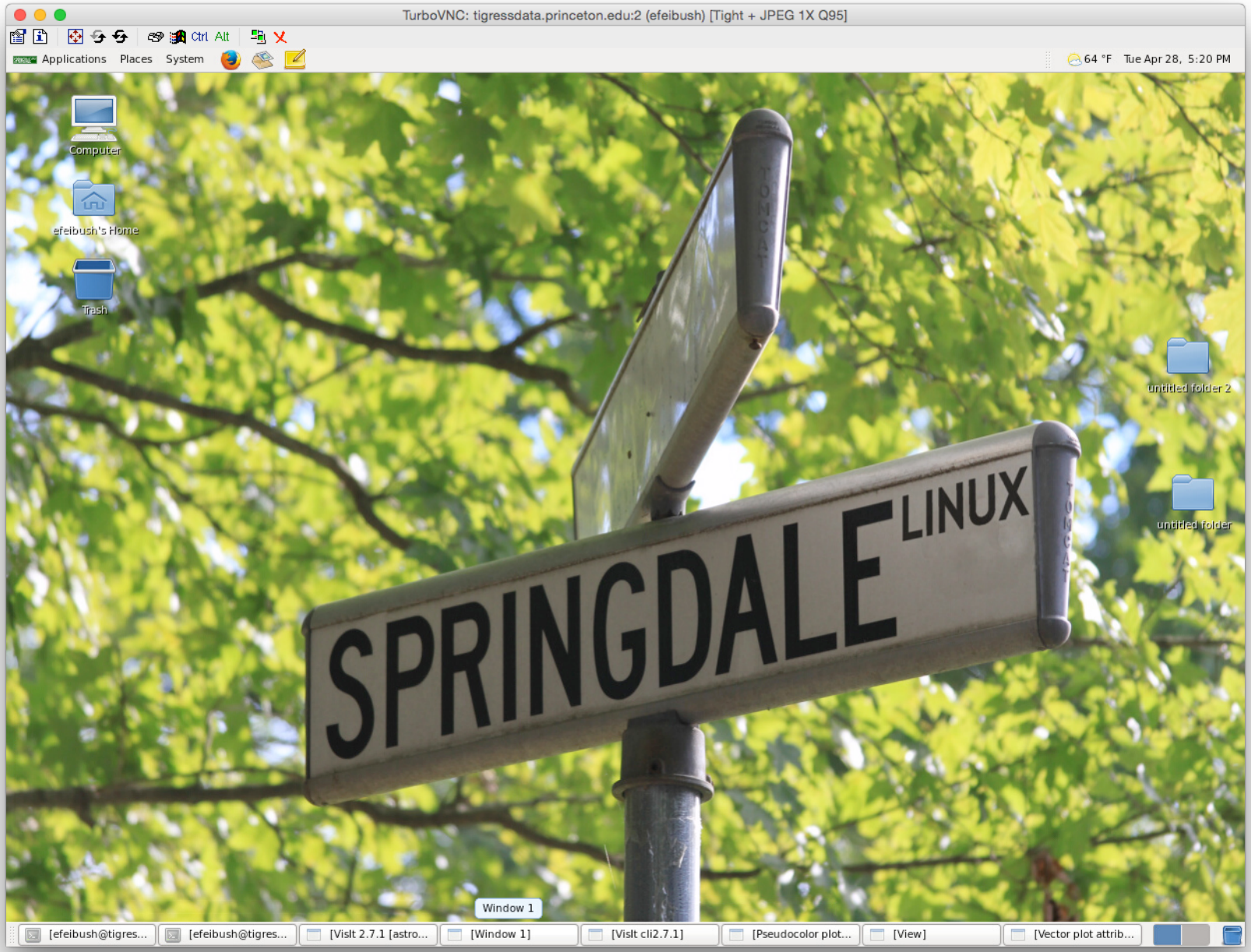
-L Enables client-server port-to-port connection.

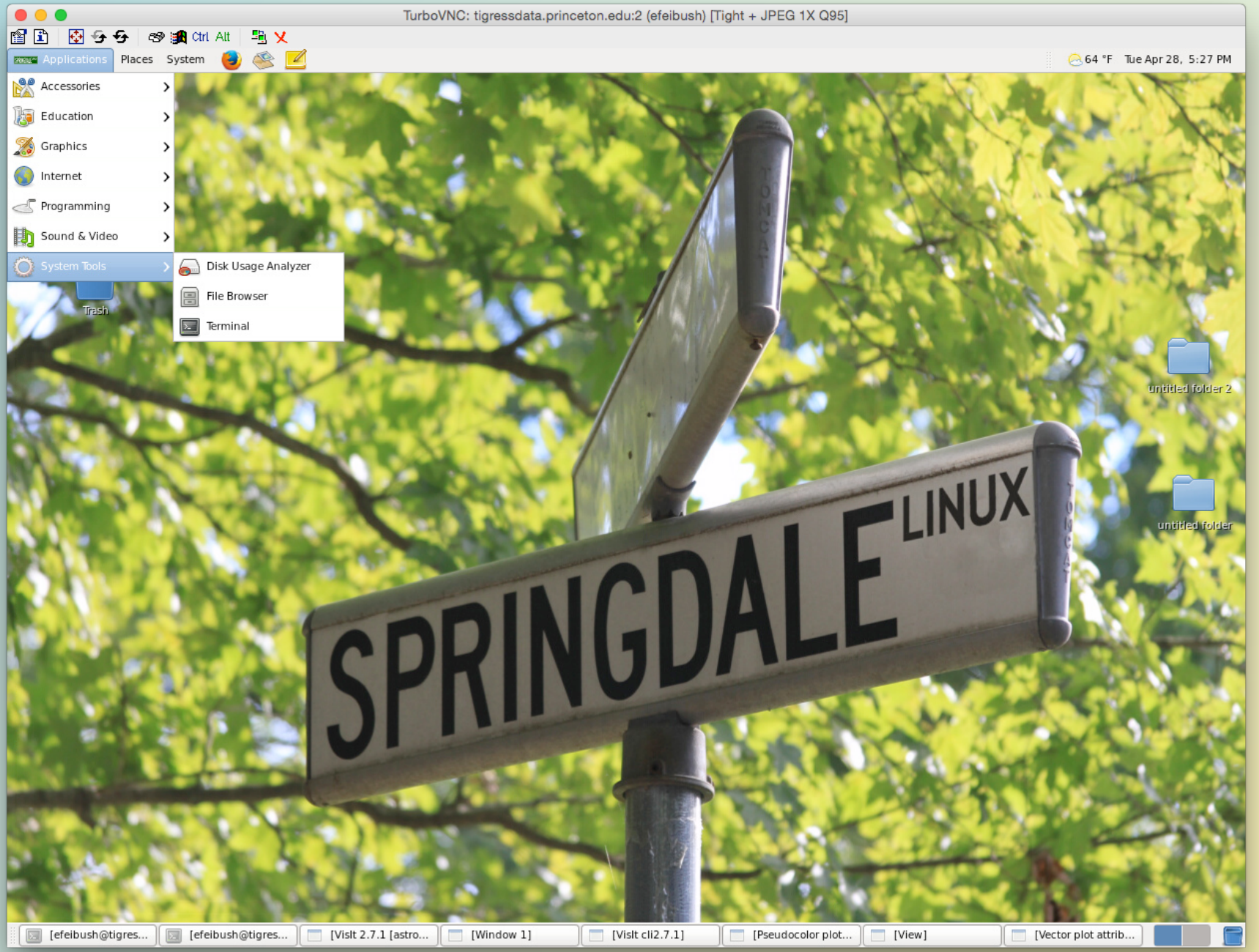
3. Run turbovnc locally

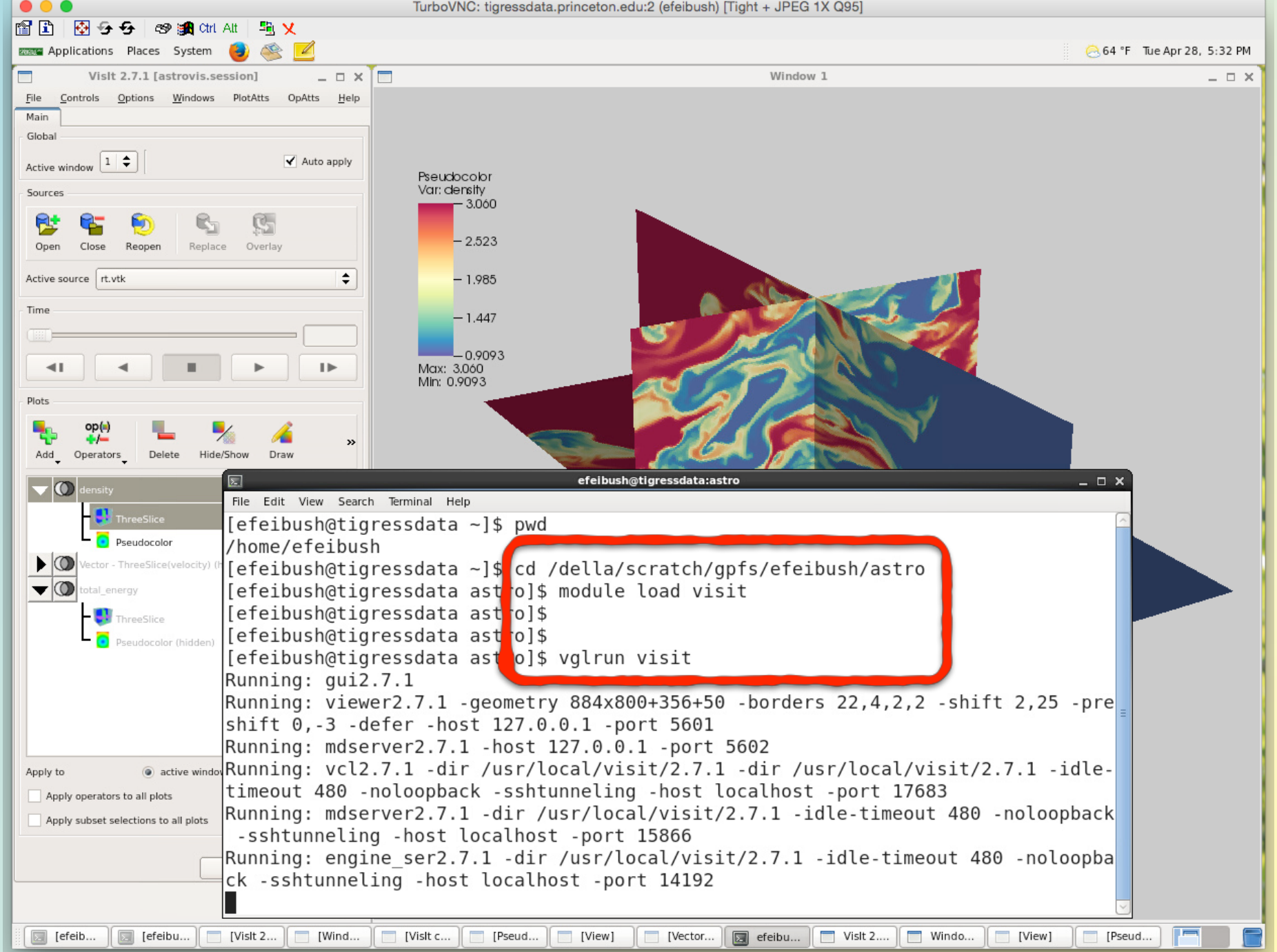


Enter your .vnc/passwd

client: turbovnc viewer




TurboVNC: tigressdata.princeton.edu:2 (efeibush) [Tight + JPEG 1X Q95]
Ctrl
Alt
Applications
Places
System
64 °F
Tue Apr 28, 5:27 PM
Accessories
Education
Graphics
Internet
Programming
Sound & Video
System Tools
Disk Usage Analyzer
File Browser
Terminal
Trash
untitled folder 2
untitled folder
SPRINGDALE
LINUX
[efeibush@tigres...
[efeibush@tigres...
[VisIt 2.7.1 [astro...
[Window 1]
[VisIt cli2.7.1]
[Pseudocolor plot...
[View]
[Vector plot attrib...


TurboVNC: tigressdata.princeton.edu:2 (efeibush) [Tight + JPEG 1X Q95]
Applications Places System
64 °F Tue Apr 28, 5:32 PM
VisIt 2.7.1 [astrovis.session]
File Controls Options Windows PlotAtts OpAtts Help
Main
Global
Active window 1
Auto apply
Sources
Open Close Reopen Replace Overlay
Active source rt.vtk
Time
Plots
Add Operators Delete Hide/Show Draw
density
ThreeSlice
Pseudocolor
Vector - ThreeSlice(velocity)
total_energy
ThreeSlice
Pseudocolor (hidden)
Apply to active window
Apply operators to all plots
Apply subset selections to all plots
Window 1
Pseudocolor
Var: density
3.060
2.523
1.985
1.447
0.9093
Max: 3.060
Min: 0.9093
efeibush@tigressdata:astro
File Edit View Search Terminal Help
[efeibush@tigressdata ~]$ pwd
/home/efeibush
[efeibush@tigressdata ~]$ cd /della/scratch/gpfs/efeibush/astro
[efeibush@tigressdata astro]$ module load visit
[efeibush@tigressdata astro]$
[efeibush@tigressdata astro]$
[efeibush@tigressdata astro]$ vglrun visit
Running: gui2.7.1
Running: viewer2.7.1 -geometry 884x800+356+50 -borders 22,4,2,2 -shift 2,25 -pre
shift 0,-3 -defer -host 127.0.0.1 -port 5601
Running: mdserver2.7.1 -host 127.0.0.1 -port 5602
Running: vcl2.7.1 -dir /usr/local/visit/2.7.1 -dir /usr/local/visit/2.7.1 -idle-
timeout 480 -noloopback -sshtunneling -host localhost -port 17683
Running: mdserver2.7.1 -dir /usr/local/visit/2.7.1 -idle-timeout 480 -noloopback
-sshtunneling -host localhost -port 15866
Running: engine_ser2.7.1 -dir /usr/local/visit/2.7.1 -idle-timeout 480 -noloopba
ck -sshtunneling -host localhost -port 14192

Parallel Rendering Set Up

***on perseus* – runs engine_par as batch job**

.cshrc or .bashrc:

module load openmpi/gcc/3.0.0/64

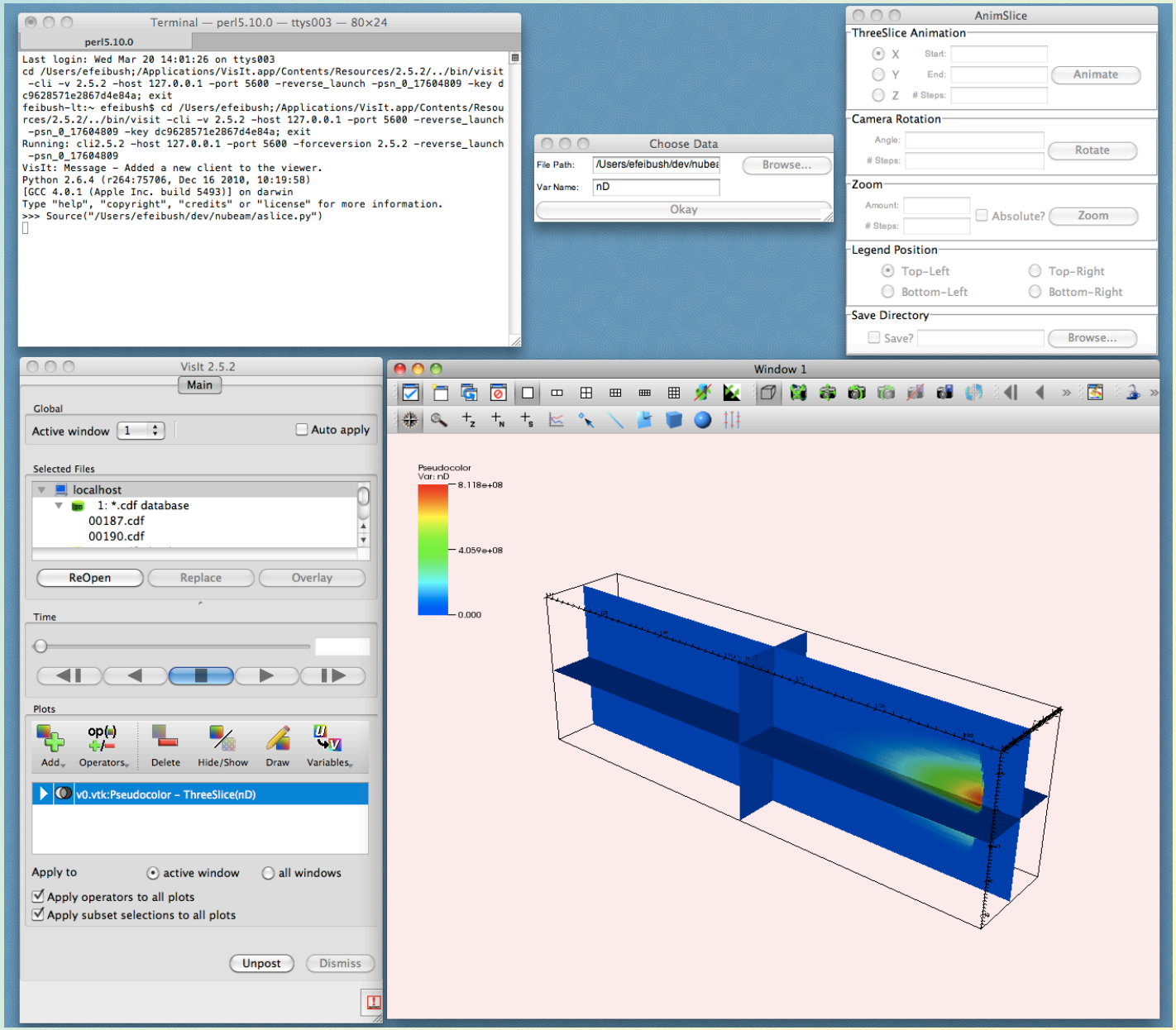
on your desktop computer or tigressdata + vnc:

~/.visit/hosts/host_princeton_perseus.xml

config file for client-server operation

Slicing & Viewing Python Package

f(x,y,z)



Try It

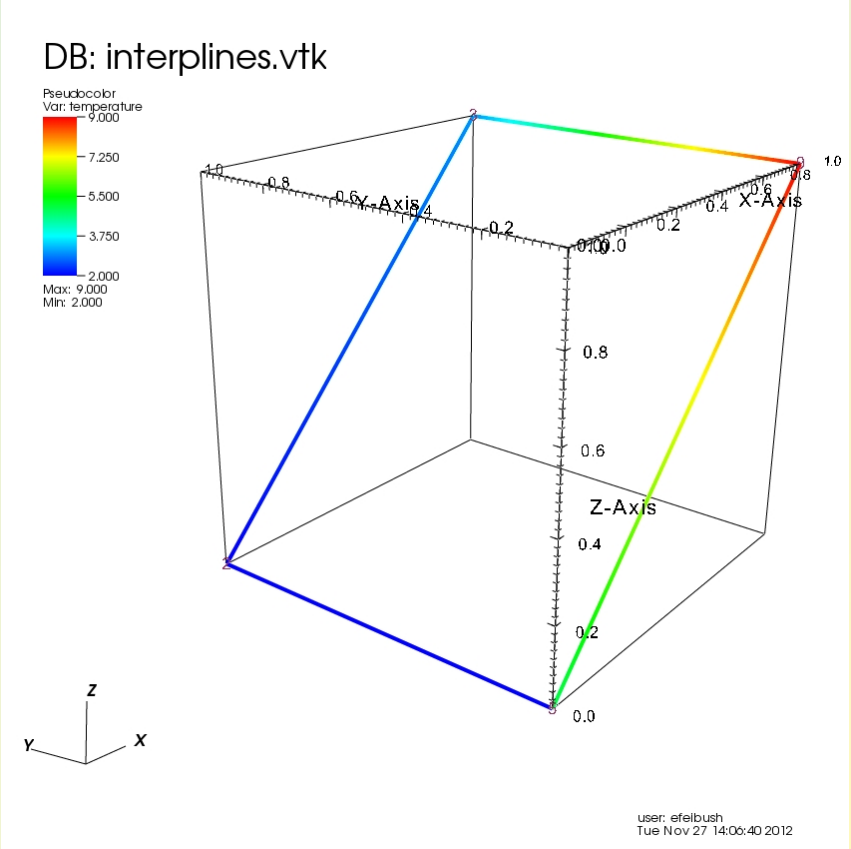
Open File interplines.vtk

Add Pseudocolor

temperature

Add Label

temperature



Example of data defined by discrete points connected with lines.

Try It

Visit Data Files:
/Volumes/dll_drive/ViSIT DATA

reboot if not on Desktop

Open File ...

/Volumes/dll-drive/ViSIT DATA

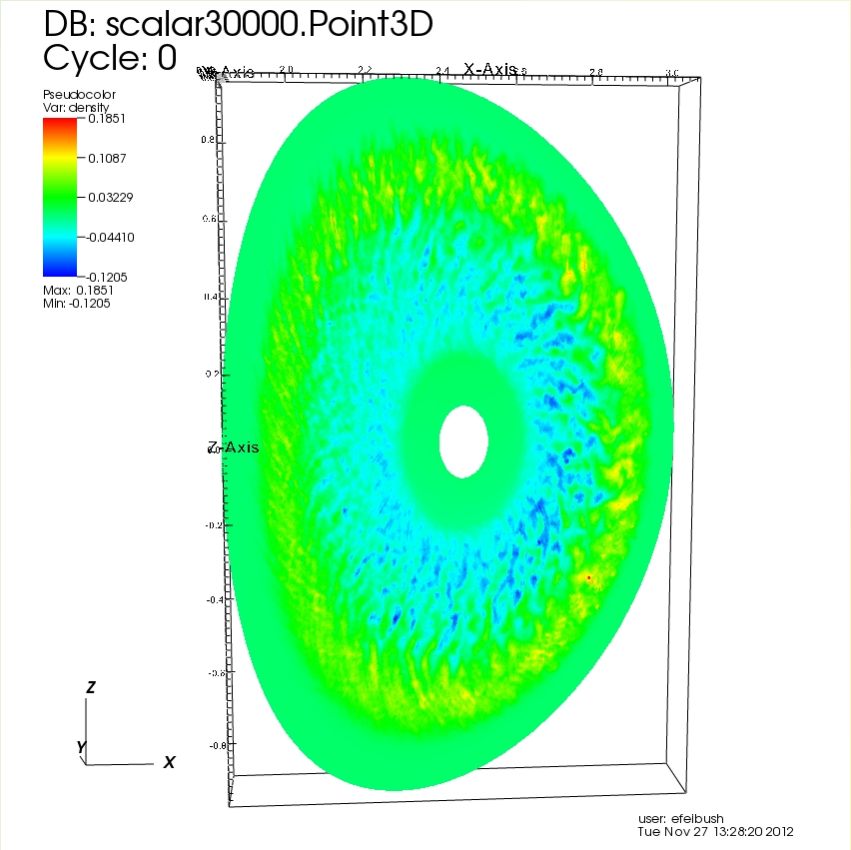
scalar30000.Point3D

Add Pseudocolor Plot

density

Attributes

Point size



Start Running VisIt

Mac

Magnifying Glass:

Spotlight: Visit

Finder

Applications

Visit.app

Windows

Start

All Programs

Visit

VisIt icon on the desktop